# IUCLID

# Data Set

| | | |
|---|---|---|
| **Existing Chemical** | : | ID: 57-11-4 |
| **EINECS Name** | : | stearic acid |
| **EC No.** | : | 200-313-4 |
| **Molecular Formula** | : | C18H36O2 |

**Producer related part**

| | | |
|---|---|---|
| **Company** | : | Epona Associates, LLC |
| **Creation date** | : | 04.12.2003 |

**Substance related part**

| | | |
|---|---|---|
| **Company** | : | Epona Associates, LLC |
| **Creation date** | : | 04.12.2003 |
| **Status** | : | |
| **Memo** | : | SOCMA MCC |
| **Printing date** | : | 05.12.2003 |
| **Revision date** | : | |
| **Date of last update** | : | 05.12.2003 |
| **Number of pages** | : | 22 |
| **Chapter (profile)** | : | Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10 |
| **Reliability (profile)** | : | Reliability: without reliability, 1, 2, 3, 4 |
| **Flags (profile)** | : | Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS |

### 1.0.1 APPLICANT AND COMPANY INFORMATION

### 1.0.2 LOCATION OF PRODUCTION SITE, IMPORTER OR FORMULATOR

### 1.0.3 IDENTITY OF RECIPIENTS

### 1.0.4 DETAILS ON CATEGORY/TEMPLATE

### 1.1.0 SUBSTANCE IDENTIFICATION

### 1.1.1 GENERAL SUBSTANCE INFORMATION

| | | |
|---|---|---|
| **Purity type** | : | |
| **Substance type** | : | organic |
| **Physical status** | : | solid |
| **Purity** | : | |
| **Colour** | : | Colorless, waxy solid |
| **Odour** | : | SLIGHT TALLOW-LIKE ODOR |
| **Source** | : | Epona Associates, LLC |
| **Reliability** | : | (2) valid with restrictions<br>Information taken from a peer-reviewed publication. |

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### 1.1.2 SPECTRA

### 1.2 SYNONYMS AND TRADENAMES

### 1.3 IMPURITIES

### 1.4 ADDITIVES

### 1.5 TOTAL QUANTITY

### 1.6.1 LABELLING

### 1.6.2 CLASSIFICATION

### 1.6.3 PACKAGING

### 1.7 USE PATTERN

### 1.7.1 DETAILED USE PATTERN

### 1.7.2 METHODS OF MANUFACTURE

### 1.8 REGULATORY MEASURES

**Type of measure** :
**Legal basis** : other: Generally Recognized as Safe

**Remark** : [Code of Federal Regulations]
[Title 21, Volume 3]
[Revised as of April 1, 2003]
From the U.S. Government Printing Office via GPO Access
[CITE: 21CFR184.1090]

TITLE 21--FOOD AND DRUGS

CHAPTER I--FOOD AND DRUG ADMINISTRATION
DEPARTMENT OF HEALTH AND HUMAN SERVICES
PART 184--DIRECT FOOD SUBSTANCES AFFIRMED AS GENERALLY RECOGNIZED AS SAFE

Subpart B--Listing of Specific Substances Affirmed as GRAS

Sec. 184.1090 Stearic acid.

(a) Stearic acid (C16H36O2, CAS Reg. No. 57-11-4) is a white to yellowish white solid. It occurs naturally as a glyceride in tallow and other animal or vegetable fats and oils and is a principal constituent of most commercially hydrogenated fats. It is produced commercially from hydrolyzed tallow derived from edible sources or from hydrolyzed, completely hydrogenated vegetable oil derived from edible sources.

(b) The ingredient meets the specifications of the Food Chemicals Codex, 3d Ed. (1981), p. 313, which is incorporated by reference, and the requirements of Sec. 172.860(b)(2) of this chapter. Copies of the Food Chemicals Codex are available from the National Academy Press, 2101 Constitution Ave. NW., Washington, DC 20418, or available for inspection at the Office of the Federal Register, 800 North Capitol Street, NW., suite 700, Washington, DC 20408.

(c) In accordance with Sec. 184.1(b)(1), the ingredient is used in food with no limitation other than current good manufacturing practice. The affirmation of this ingredient as generally recognized as safe (GRAS) as a direct human food ingredient is based upon the following current good manufacturing practice conditions of use:

(1) The ingredient is used as a flavoring agent and adjuvant as

defined in Sec. 170.3(o)(12) of this chapter.
(2) The ingredient is used in foods at levels not to exceed current good manufacturing practice.
(d) Prior sanctions for this ingredient different from the uses established in this section do not exist or have been waived.

[48 FR 52445, Nov. 18, 1983, as amended at 50 FR 49536, Dec. 3, 1985]

**Reliability** : (1) valid without restriction
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**1.8.1 OCCUPATIONAL EXPOSURE LIMIT VALUES**

**1.8.2 ACCEPTABLE RESIDUES LEVELS**

**1.8.3 WATER POLLUTION**

**1.8.4 MAJOR ACCIDENT HAZARDS**

**1.8.5 AIR POLLUTION**

**1.8.6 LISTINGS E.G. CHEMICAL INVENTORIES**

**1.9.1 DEGRADATION/TRANSFORMATION PRODUCTS**

**1.9.2 COMPONENTS**

**1.10 SOURCE OF EXPOSURE**

**1.11 ADDITIONAL REMARKS**

**1.12 LAST LITERATURE SEARCH**

**1.13 REVIEWS**

### 2.1 MELTING POINT

| | | |
|---|---|---|
| **Value** | : | = 69 - 70 °C |
| **Sublimation** | : | |
| **Method** | : | |
| **Year** | : | 1982 |
| **GLP** | : | no data |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Source** | : | Epona Associates, LLC |
| **Reliability** | : | (2) valid with restrictions<br>Information taken from a peer-reviewed publication. |
| **Flag** | : | Critical study for SIDS endpoint |

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### 2.2 BOILING POINT

| | | |
|---|---|---|
| **Value** | : | = 383 °C at 1013 hPa |
| **Decomposition** | : | |
| **Method** | : | |
| **Year** | : | |
| **GLP** | : | no data |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Source** | : | Epona Associates, LLC |
| **Reliability** | : | (2) valid with restrictions<br>Information taken from a peer-reviewed publication. |
| **Flag** | : | Critical study for SIDS endpoint |

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### 2.3 DENSITY

#### 2.3.1 GRANULOMETRY

### 2.4 VAPOUR PRESSURE

| | | |
|---|---|---|
| **Value** | : | = 1.33 hPa at 173.7 °C |
| **Decomposition** | : | |
| **Method** | : | |
| **Year** | : | 1969 |
| **GLP** | : | no data |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Source** | : | Epona Associates, LLC |
| **Reliability** | : | (2) valid with restrictions<br>Information taken from a peer-reviewed publication. |
| **Flag** | : | Critical study for SIDS endpoint |

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### 2.5 PARTITION COEFFICIENT

| | | |
|---|---|---|
| **Partition coefficient** | : | octanol-water |
| **Log pow** | : | = 8.42 at °C |
| **pH value** | : | |
| **Method** | : | |
| **Year** | : | |
| **GLP** | : | no data |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Source** | : | Epona Associates, LLC |
| **Reliability** | : | (2) valid with restrictions<br>Information taken from a peer-reviewed publication. |

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### 2.6.1 SOLUBILITY IN DIFFERENT MEDIA

| | | |
|---|---|---|
| **Solubility in** | : | Water |
| **Value** | : | = .568 mg/l at 25 °C |
| **pH value** | : | |
| **concentration** | : | at °C |
| **Temperature effects** | : | |
| **Examine different pol.** | : | |
| **pKa** | : | at 25 °C |
| **Description** | : | |
| **Stable** | : | |
| **Deg. product** | : | |
| **Method** | : | other: measured |
| **Year** | : | 1966 |
| **GLP** | : | no data |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Result** | : | Water solubility = .0001 mg/L at 30 deg C |
| **Reliability** | : | (2) valid with restrictions<br>Information taken from a peer-reviewed publication. |

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### 2.6.2 SURFACE TENSION

### 2.7 FLASH POINT

### 2.8 AUTO FLAMMABILITY

### 2.9 FLAMMABILITY

### 2.10 EXPLOSIVE PROPERTIES

### 2.11 OXIDIZING PROPERTIES

### 2.12 DISSOCIATION CONSTANT

## 2.13 VISCOSITY

## 2.14 ADDITIONAL REMARKS

### 3.1.1 PHOTODEGRADATION

| | | |
|---|---|---|
| **Type** | : | air |
| **Light source** | : | |
| **Light spectrum** | : | nm |
| **Relative intensity** | : | based on intensity of sunlight |
| **DIRECT PHOTOLYSIS** | | |
| **Halflife t1/2** | : | = .5 day(s) |
| **Degradation** | : | % after |
| **Quantum yield** | : | |
| **Deg. product** | : | |
| **Method** | : | other (calculated) |
| **Year** | : | 2003 |
| **GLP** | : | no |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |

| | | |
|---|---|---|
| **Method** | : | Estimated using AopWin v1.91 |
| **Result** | : | Atmospheric Oxidation (25 deg C) [AopWin v1.91]:<br>Hydroxyl Radicals Reaction:<br>OVERALL OH Rate Constant = 22.4804 E-12 cm3/molecule-sec<br>Half-Life = 0.476 Days (12-hr day; 1.5E6 OH/cm3)<br>Half-Life = 5.710 Hrs<br>Ozone Reaction:<br>No Ozone Reaction Estimation |
| **Source** | : | Epona Associates, LLC |
| **Reliability** | : | (2) valid with restrictions |
| **Flag** | : | Critical study for SIDS endpoint |

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| | | |
|---|---|---|
| **Type** | : | air |
| **Light source** | : | |
| **Light spectrum** | : | nm |
| **Relative intensity** | : | based on intensity of sunlight |
| **DIRECT PHOTOLYSIS** | | |
| **Halflife t1/2** | : | = 17 hour(s) |
| **Degradation** | : | % after |
| **Quantum yield** | : | |
| **Deg. product** | : | |
| **Method** | : | |
| **Year** | : | |
| **GLP** | : | no data |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |

| | | |
|---|---|---|
| **Result** | : | Vapor phase stearic acid is degraded in the atmosphere by reaction with photochemically-produced hydroxyl radicals with a half-life of about 17 hours. |
| **Source** | : | Epona Associates, LLC |
| **Reliability** | : | (2) valid with restrictions<br>Information taken from a peer-reviewed publication. |

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### 3.1.2 STABILITY IN WATER

### 3.1.3 STABILITY IN SOIL

### 3.2.1 MONITORING DATA

### 3.2.2 FIELD STUDIES

### 3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

| | | |
|---|---|---|
| **Type** | : | fugacity model level III |
| **Media** | : | |
| **Air** | : | % (Fugacity Model Level I) |
| **Water** | : | % (Fugacity Model Level I) |
| **Soil** | : | % (Fugacity Model Level I) |
| **Biota** | : | % (Fugacity Model Level II/III) |
| **Soil** | : | % (Fugacity Model Level II/III) |
| **Method** | : | other: modeling |
| **Year** | : | 2003 |
| **Method** | : | EPI v3.11 |
| **Result** | : | Level III Fugacity Model:<br>Mass Amount Half-Life Emissions<br>(percent) (hr) (kg/hr)<br>Air 0.676 11.4 1000<br>Water 7.19 360 1000<br>Soil 28.9 360 1000<br>Sediment 63.3 1.44e+003 0<br>Persistence Time: 640 hr |
| **Source** | : | Epona Associates, LLC |
| **Reliability** | : | (2) valid with restrictions |
| **Flag** | : | Critical study for SIDS endpoint |

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### 3.3.2 DISTRIBUTION

### 3.4 MODE OF DEGRADATION IN ACTUAL USE

### 3.5 BIODEGRADATION

| | | |
|---|---|---|
| **Type** | : | aerobic |
| **Inoculum** | : | activated sludge |
| **Contact time** | : | |
| **Degradation** | : | = 77 (±) % after 28 day(s) |
| **Result** | : | readily biodegradable |
| **Kinetic of testsubst.** | : | 10 day(s) = 65 %<br>14 day(s) = 69 %<br>28 day(s) = 77 %<br>%<br>% |
| **Deg. product** | : | |
| **Method** | : | other: BOD test |
| **Year** | : | 1983 |
| **GLP** | : | no data |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Remark** | : | Results are an average of 11 participating laboratories. |

**Result** : 65, 69 and 77 % degradation after 10, 14 and 28 days, respectively.
**Source** : Epona Associates, LLC
**Reliability** : (2) valid with restrictions
Information taken from a peer-reviewed publication.
05.12.2003 (7)

**Type** : aerobic
**Inoculum** : activated sludge
**Concentration** : 100 g/l related to Test substance
related to
**Contact time** : 5 day(s)
**Degradation** : (±) % after
**Result** : readily biodegradable
**Deg. product** :
**Method** : other: BOD5
**Year** : 1985
**GLP** : no data
**Test substance** : as prescribed by 1.1 - 1.4

**Result** : Rate: .0088 1/HR

Half-Life [Days]: 3.3
**Source** : Epona Associates, LLC
**Test condition** : BOD test conducted at 20 deg C.
**Reliability** : (2) valid with restrictions
Information taken from a peer-reviewed publication.
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**Type** : aerobic
**Inoculum** : other: sewage sludge
**Contact time** : 21 day(s)
**Degradation** : = 95 (±) % after 21 day(s)
**Result** : readily biodegradable
**Deg. product** :
**Method** : other: Sturm $CO_2$ evolution
**Year** : 1984
**GLP** : no data
**Test substance** : as prescribed by 1.1 - 1.4

**Source** : Epona Associates, LLC
**Reliability** : (2) valid with restrictions
Information taken from a peer-reviewed publication.
**Flag** : Critical study for SIDS endpoint
05.12.2003 (13)

**Type** : aerobic
**Inoculum** : activated sludge
**Contact time** :
**Degradation** : (±) % after
**Result** : readily biodegradable
**Deg. product** :
**Method** : other: Warburg
**Year** : 1973
**GLP** : no data
**Test substance** : as prescribed by 1.1 - 1.4

**Result** : Rate: .0077; .0052; .00217

Rate Units: 1/HR

Half-Life [Days]: 3.75; 5.55; 10.7
**Source** : Epona Associates, LLC

| | | |
|---|---|---|
| **Test condition** | : | Test Method: WARBURG<br>Oxygen Condition: AEROBIC<br>Analysis Method: 02 UPTAKE<br>Inoculum: ACTIVATED SLUDGE<br>Temperature [øC]: 20; 25; 30 |
| **Reliability** | : | (2) valid with restrictions<br>Information taken from a peer-reviewed publication. |

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## 3.6 BOD5, COD OR BOD5/COD RATIO

## 3.7 BIOACCUMULATION

## 3.8 ADDITIONAL REMARKS

## 4.1 ACUTE/PROLONGED TOXICITY TO FISH

| | | |
|---|---|---|
| **Type** | : | static |
| **Species** | : | Oncorhynchus kisutch (Fish, fresh water, marine) |
| **Exposure period** | : | 96 hour(s) |
| **Unit** | : | µg/l |
| **LC50** | : | = 12000 measured/nominal |
| **Method** | : | |
| **Year** | : | 1977 |
| **GLP** | : | no data |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Source** | : | Epona Associates, LLC |
| **Test substance** | : | "pure" |
| **Reliability** | : | (2) valid with restrictions |
| **Flag** | : | Critical study for SIDS endpoint |

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## 4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

## 4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

## 4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

## 4.5.1 CHRONIC TOXICITY TO FISH

## 4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

## 4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS

## 4.6.2 TOXICITY TO TERRESTRIAL PLANTS

## 4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS

## 4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES

## 4.7 BIOLOGICAL EFFECTS MONITORING

## 4.8 BIOTRANSFORMATION AND KINETICS

### 4.9 ADDITIONAL REMARKS

## 5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

## 5.1.1 ACUTE ORAL TOXICITY

| | | |
|---|---|---|
| **Type** | : | LD50 |
| **Value** | : | = 4600 mg/kg bw |
| **Species** | : | rat |
| **Strain** | : | |
| **Sex** | : | |
| **Number of animals** | : | |
| **Vehicle** | : | |
| **Doses** | : | |
| **Method** | : | |
| **Year** | : | |
| **GLP** | : | no data |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Source** | : | Epona Associates, LLC |
| **Reliability** | : | (2) valid with restrictions<br>Information taken from a peer-reviewed publication. |

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| | | |
|---|---|---|
| **Type** | : | LD100 |
| **Value** | : | = 14286 - mg/kg bw |
| **Species** | : | human |
| **Strain** | : | |
| **Sex** | : | |
| **Number of animals** | : | |
| **Vehicle** | : | |
| **Doses** | : | |
| **Method** | : | |
| **Year** | : | 1976 |
| **GLP** | : | no data |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Result** | : | Minimum/Potential Fatal Human Dose:<br>1. 1= PRACTICALLY NONTOXIC: PROBABLE ORAL LETHAL DOSE (HUMAN) MORE THAN 1<br>QT (2.2 LB) FOR 70 KG PERSON (150 LB). |
| **Source** | : | Epona Associates, LLC |
| **Reliability** | : | (2) valid with restrictions<br>Information taken from a peer-reviewed publication. |

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## 5.1.2 ACUTE INHALATION TOXICITY

## 5.1.3 ACUTE DERMAL TOXICITY

## 5.1.4 ACUTE TOXICITY, OTHER ROUTES

## 5.2.1 SKIN IRRITATION

## 5.2.2 EYE IRRITATION

## 5.3 SENSITIZATION

## 5.4 REPEATED DOSE TOXICITY

| | | |
|---|---|---|
| **Type** | : | Sub-chronic |
| **Species** | : | rat |
| **Sex** | : | |
| **Strain** | : | |
| **Route of admin.** | : | oral feed |
| **Exposure period** | : | 24 weeks |
| **Frequency of treatm.** | : | |
| **Post exposure period** | : | |
| **Doses** | : | 50g/kg/day |
| **Control group** | : | |
| **Method** | : | |
| **Year** | : | |
| **GLP** | : | no data |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Result** | : | Rats fed 50 g/kg/day stearic acid for 24 weeks developed reversible lipogranulomas in adipose tissue. No significant pathological lesions were observed in rats fed 3000 ppm stearic acid orally for about 30 weeks, but anorexia, increased mortality, and a greater incidence of pulmonary infection were observed. Stearic acid is one of the least effective fatty acids in producing hyperlipemia, but the most potent in diminishing blood clotting time. |
| **Source** | : | Epona Associates, LLC |
| **Reliability** | : | (2) valid with restrictions<br>Information taken from a peer-reviewed publication. |

05.12.2003 (2)

| | | |
|---|---|---|
| **Type** | : | Sub-acute |
| **Species** | : | rat |
| **Sex** | : | |
| **Strain** | : | |
| **Route of admin.** | : | oral feed |
| **Exposure period** | : | 6 or 9 weeks |
| **Frequency of treatm.** | : | |
| **Post exposure period** | : | |
| **Doses** | : | 5 or 6% |
| **Control group** | : | |
| **Result** | : | Rats fed 5% stearic acid as part of a high-fat diet for 6 weeks, or 6% stearic acid for 9 weeks, showed a decreased blood clotting time and hyperlipemia. |
| **Source** | : | Epona Associates, LLC |
| **Reliability** | : | (2) valid with restrictions<br>Information taken from a peer-reviewed publication. |

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| | | |
|---|---|---|
| **Type** | : | Sub-acute |
| **Species** | : | mouse |

| | | |
|---|---|---|
| **Sex** | : | |
| **Strain** | : | |
| **Route of admin.** | : | oral feed |
| **Exposure period** | : | 3 weeks |
| **Frequency of treatm.** | : | |
| **Post exposure period** | : | |
| **Doses** | : | 5 to 50% |
| **Control group** | : | |
| **Method** | : | |
| **Year** | : | |
| **GLP** | : | no data |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Result** | : | When diets containing 5 to 50% stearic acid (as the monoglyceride) were fed to weanling mice for 3 weeks, depression of weight gain was seen above the 10% dietary level. Mortality occurred only with the 50% diet. The effects were less noticeable in adult mice. |
| **Source** | : | Epona Associates, LLC |
| **Reliability** | : | (2) valid with restrictions<br>Information taken from a peer-reviewed publication. |

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## 5.5 GENETIC TOXICITY 'IN VITRO'

## 5.6 GENETIC TOXICITY 'IN VIVO'

## 5.7 CARCINOGENICITY

## 5.8.1 TOXICITY TO FERTILITY

## 5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

## 5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

## 5.9 SPECIFIC INVESTIGATIONS

## 5.10 EXPOSURE EXPERIENCE

## 5.11 ADDITIONAL REMARKS

## 6.1 ANALYTICAL METHODS

## 6.2 DETECTION AND IDENTIFICATION

## 7.1 FUNCTION

## 7.2 EFFECTS ON ORGANISMS TO BE CONTROLLED

## 7.3 ORGANISMS TO BE PROTECTED

## 7.4 USER

## 7.5 RESISTANCE

## 8.1 METHODS HANDLING AND STORING

## 8.2 FIRE GUIDANCE

## 8.3 EMERGENCY MEASURES

## 8.4 POSSIB. OF RENDERING SUBST. HARMLESS

## 8.5 WASTE MANAGEMENT

## 8.6 SIDE-EFFECTS DETECTION

## 8.7 SUBSTANCE REGISTERED AS DANGEROUS FOR GROUND WATER

## 8.8 REACTIVITY TOWARDS CONTAINER MATERIAL

(1) Bidleman TF (1988) Environ Sci Technol 22: 361-367 (1988). Cited in BiblioLine.

(2) Clayton, G.D., F.E. Clayton (eds.) Patty's Industrial Hygiene and Toxicology. Volumes 2A, 2B, 2C, 2D, 2E, 2F: Toxicology. 4th ed. New York, NY: John Wiley & Sons Inc., 1993-1994. 3568. Cited in BiblioLine

(3) Daubert TE, Danner RP (1989) Physical and Thermodynamic Properties of Pure Chemicals: Data Domination. Design Inst Phys Prop Data, Amer Inst Chem Eng. NY,NY: Hemisphere Pub. Corp 4 Vol (1989). Cited in BiblioLine.

(4) Gosselin, R.E., H.C. Hodge, R.P. Smith, and M.N. Gleason (1976) Clinical Toxicology of Commercial Products. 4th ed. Baltimore: Williams and Wilkins, 1976.,p. II-135. Cited in BiblioLine.

(5) HSDB SUBSET [Hazardous Substances Data Bank]

(6) Johnson RW, Daniels RW (1993) Kirk-Othmer Encycl Chem Tech. 4th ed. NY,NY: John Wiley and Sons 5: 147-158 (1993). Cited in BiblioLine.

(7) King, E.F.; Painter, H.A. (1983) RING-TEST PROGRAM 1981-1982. ASSESSMENT OF BIODEGRADABILITY OF CHEMICALS IN WATER BY MANOMETRIC RESPIROMETRY. COMM. EUR. COMMUNITIES, EUR 8631. 31 PP, 1983 CIS Record ID.: BD-0000218

(8) Leach, J.M. and A.N. Thakore (1977) Compounds Toxic to Fish Pulp Mill Waste Streams Progress in Water Technology, 9: 787-798 CIS Record ID.: AQ-0132049.

(9) Leo, A.J. (1978) Report on the Calculation of Octanol/Water Log P Values for Structures in EPA Files.
CIS Record ID : IS-0000416. BiblioLine © 1997-2003, NISC International, Inc.

(10) Meylan WM, Howard PH (1993) Chemosphere 26: 2293-99 (1993). Cited in BiblioLine.

(11) Novak, J.T. and Kraus, D.L. (1973) DEGRADATION OF LONG CHAIN FATTY ACIDS BY ACTIVATED SLUDGE. Water Research, 7: 843-51, 1973 ISSN: 0043-1354 CIS Record ID.: BD-0000208.

(12) Robb ID (1966) Aust J Chem 19: 2281-84 (1966) Cited in BiblioLine © 1997-2003, NISC International, Inc.

(13) Ruffo, C.; Galli, E.; Arpino, A. (1984) COMPARISON OF METHODS FOR THE BIODEGRADABILITY OF SOLUBLE AND INSOLUBLE ORGANOCHEMICALS. Ecotoxicology and Environmental Safety, 8: 275-9, 1984 CIS Record ID.: BD-0000209. BiblioLine © 1997-2003, NISC International, Inc.

(14) Urano, K. and Saito, M. (1985) BIODEGRADABILITY OF SURFACTANTS AND INHIBITION OF SURFACTANTS TO BIODEGRADATION OF OTHER POLLUTANTS, Chemosphere, 14: 1333-42, 1985
CIS Record ID.: BD-0000210. BiblioLine © 1997-2003, NISC International, Inc.

(15) Weast, R.C. (1969) Chemical Rubber Company Handbook of Chemistry and Physics. 50th Ed, CRC Press, Inc. Cleveland, Ohio, 1969 CIS Record ID.: IS-0000414. BiblioLine © 1997-2003, NISC International, Inc.

(16) Windholz, M. (1982)The Merck Index, 9th Edition Merck and Company, Inc., Rahway, NJ, 1982. CIS Record ID.: IS-0000412 BiblioLine © 1997-2003, NISC International, Inc.

## 10.1 END POINT SUMMARY

## 10.2 HAZARD SUMMARY

## 10.3 RISK ASSESSMENT

# IUCLID

# Data Set

| | | |
|---|---|---|
| **Existing Chemical** | : | ID: 7446-70-0 |
| **CAS No.** | : | 7446-70-0 |
| **EINECS Name** | : | aluminium chloride |
| **EC No.** | : | 231-208-1 |
| **TSCA Name** | : | Aluminum chloride (AlCl3) |
| **Molecular Formula** | : | AlCl3 |

**Producer related part**

| | | |
|---|---|---|
| **Company** | : | Epona Associates, LLC |
| **Creation date** | : | 28.11.2003 |

**Substance related part**

| | | |
|---|---|---|
| **Company** | : | Epona Associates, LLC |
| **Creation date** | : | 28.11.2003 |
| **Status** | : | |
| **Memo** | : | MCC |
| **Printing date** | : | 04.12.2003 |
| **Revision date** | : | |
| **Date of last update** | : | 04.12.2003 |
| **Number of pages** | : | 18 |
| **Chapter (profile)** | : | Chapter: 2.1, 2.2, 2.4, 2.5, 2.6.1, 3.1.1, 3.1.2, 3.3.1, 3.5, 4.1, 4.2, 4.3, 5.1.1, 5.1.2, 5.1.3, 5.1.4, 5.4, 5.5, 5.6, 5.8.1, 5.8.2 |
| **Reliability (profile)** | : | Reliability: without reliability, 1, 2, 3, 4 |
| **Flags (profile)** | : | Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS |

### 2.1 MELTING POINT

| | | |
|---|---|---|
| **Value** | : | = 190 °C |
| **Sublimation** | : | |
| **Method** | : | |
| **Year** | : | 1969 |
| **GLP** | : | no |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Source** | : | Epona Asociates, LLC |
| **Reliability** | : | (2) valid with restrictions<br>Information taken from a peer-reviewed publication. |
| **Flag** | : | Critical study for SIDS endpoint |

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### 2.2 BOILING POINT

| | | |
|---|---|---|
| **Value** | : | = 182 °C at 1002 |
| **Decomposition** | : | |
| **Method** | : | |
| **Year** | : | 1969 |
| **GLP** | : | no |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Source** | : | Epona Asociates, LLC |
| **Reliability** | : | (2) valid with restrictions<br>Information taken from a peer-reviewed publication. |
| **Flag** | : | Critical study for SIDS endpoint |

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### 2.4 VAPOUR PRESSURE

| | | |
|---|---|---|
| **Value** | : | = 1.38 hPa at 100 °C |
| **Decomposition** | : | |
| **Method** | : | |
| **Year** | : | 1969 |
| **GLP** | : | no |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Source** | : | Epona Asociates, LLC |
| **Reliability** | : | (2) valid with restrictions<br>Information taken from a peer-reviewed publication. |
| **Flag** | : | Critical study for SIDS endpoint |

28.11.2003 (28)

### 2.5 PARTITION COEFFICIENT

| | | |
|---|---|---|
| **Partition coefficient** | : | octanol-water |
| **Log pow** | : | = 1.26 at °C |
| **pH value** | : | |
| **Method** | : | other (calculated) |
| **Year** | : | 2003 |
| **GLP** | : | no |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |

| | | |
|---|---|---|
| **Method** | : | Modeled data; estimated using KOWWIN v 1.67 |
| **Source** | : | Epona Asociates, LLC |
| **Reliability** | : | (2) valid with restrictions |
| **Flag** | : | Critical study for SIDS endpoint |

04.12.2003

### 2.6.1 SOLUBILITY IN DIFFERENT MEDIA

| | | |
|---|---|---|
| **Solubility in** | : | Water |
| **Value** | : | = 450 g/l at 20 °C |
| **pH value** | : | = 2.4 |
| **concentration** | : | 100 g/l at 20 °C |
| **Temperature effects** | : | |
| **Examine different pol.** | : | |
| **pKa** | : | at 25 °C |
| **Description** | : | |
| **Stable** | : | |
| **Deg. product** | : | |
| **Method** | : | |
| **Year** | : | 1988 |
| **GLP** | : | no data |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| | | |
| **Source** | : | BASF AG Ludwigshafen |
| **Reliability** | : | (4) not assignable<br>Original study not reviewed. |
| **Flag** | : | Critical study for SIDS endpoint |

04.12.2003 (3)

### 3.1.1 PHOTODEGRADATION

| | | |
|---|---|---|
| **Type** | : | air |
| **Light source** | : | |
| **Light spectrum** | : | nm |
| **Relative intensity** | : | based on intensity of sunlight |
| **Deg. product** | : | |
| **Method** | : | |
| **Year** | : | 2003 |
| **GLP** | : | no |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Method** | : | Estimated using AopWin v1.91 |
| **Result** | : | Atmospheric Oxidation (25 deg C) [AopWin v1.91]:<br>Hydroxyl Radicals Reaction:<br>OVERALL OH Rate Constant = 0.0000 E-12 cm3/molecule-sec<br>Half-Life = -------<br>Ozone Reaction:<br>No Ozone Reaction Estimation |
| **Source** | : | Epona Asociates, LLC |
| **Reliability** | : | (2) valid with restrictions |

04.12.2003

### 3.1.2 STABILITY IN WATER

| | | |
|---|---|---|
| **Type** | : | abiotic |
| **t1/2 pH4** | : | at °C |
| **t1/2 pH7** | : | at °C |
| **t1/2 pH9** | : | at °C |
| **Deg. product** | : | |
| **Method** | : | |
| **Year** | : | 2000 |
| **GLP** | : | no data |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Remark** | : | The material is unstable in water, 700g/l @ 15 deg C.<br>There is an immediate violent reaction yielding HCl gas. |
| **Source** | : | Whyte Chemicals Ltd London |
| **Reliability** | : | (4) not assignable<br>Original study not reviewed. |

04.12.2003 (12)

### 3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

| | | |
|---|---|---|
| **Type** | : | fugacity model level III |
| **Media** | : | |
| **Air** | : | % (Fugacity Model Level I) |
| **Water** | : | % (Fugacity Model Level I) |
| **Soil** | : | % (Fugacity Model Level I) |
| **Biota** | : | % (Fugacity Model Level II/III) |
| **Soil** | : | % (Fugacity Model Level II/III) |
| **Method** | : | other: modeling |
| **Year** | : | 2003 |
| **Method** | : | Estimated using EPI SUMMARY (v3.11) |
| **Remark** | : | The material will decompose 100% in the presence of water to |

give aluminium oxide and HCl gas (ECB IULCID, 2000).

**Result** : Level III Fugacity Model:

| | Mass Amount (percent) | Half-Life (hr) | Emissions (kg/hr) |
|---|---|---|---|
| Air | 5.39e-006 | 1e+005 | 1000 |
| Water | 39.8 | 360 | 1000 |
| Soil | 60.1 | 360 | 1000 |
| Sediment | 0.0767 | 1.44e+003 | 0 |

Persistence Time: 431 hr

**Source** : Epona Asociates, LLC
**Reliability** : (2) valid with restrictions
**Flag** : Critical study for SIDS endpoint
04.12.2003

## 3.5 BIODEGRADATION

**Deg. product** :
**Method** : other: modeling
**Year** : 2003
**GLP** : no
**Test substance** : as prescribed by 1.1 - 1.4

**Remark** : The material decompose 100% in the presence of water to give aluminium oxide and HCl gas (ECB IUCLID, 2000).

**Result** : Probability of Rapid Biodegradation (BIOWIN v4.01):
Linear Model : 0.6841
Non-Linear Model : 0.7531
Expert Survey Biodegradation Results:
Ultimate Survey Model: 2.9045 (weeks)
Primary Survey Model : 3.6554 (days-weeks )
Readily Biodegradable Probability (MITI Model):
Linear Model : 0.3155
Non-Linear Model : 0.2102

**Source** : Epona Asociates, LLC
**Reliability** : (2) valid with restrictions
**Flag** : Critical study for SIDS endpoint
04.12.2003

## 4.1 ACUTE/PROLONGED TOXICITY TO FISH

| | | |
|---|---|---|
| **Type** | : | |
| **Species** | : | Brachydanio rerio (Fish, fresh water) |
| **Exposure period** | : | 48 hour(s) |
| **Unit** | : | mg/l |
| **LC50** | : | = 80 |
| **Method** | : | |
| **Year** | : | 1985 |
| **GLP** | : | no data |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Source** | : | Epona Asociates, LLC |
| **Reliability** | : | (2) valid with restrictions |

28.11.2003 (9)

| | | |
|---|---|---|
| **Type** | : | |
| **Species** | : | Gambusia affinis (Fish, fresh water) |
| **Exposure period** | : | 24 hour(s) |
| **Unit** | : | mg/l |
| **LC50** | : | = 29.6 calculated |
| **Method** | : | other |
| **Year** | : | 1957 |
| **GLP** | : | no |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Remark** | : | EC50 value calculated by AQUIRE staff based on data in paper |
| **Source** | : | Epona Asociates, LLC |
| **Test condition** | : | Water Parameters:<br>Temperature: 20 (min. value); 21 (max. value) C<br>Alkalinity (mg/l CaCO3): <100 (mean value) mg/L CaCO3 (<br>pH 4.3 (min. value); 7.2 (max. value) |
| **Reliability** | : | (2) valid with restrictions<br>Information taken from a peer-reviewed publication. |

28.11.2003 (27)

| | | |
|---|---|---|
| **Type** | : | |
| **Species** | : | Oncorhynchus mykiss (Fish, fresh water) |
| **Exposure period** | : | 96 hour(s) |
| **Unit** | : | mg/l |
| **LC50** | : | = 8.6 |

28.11.2003 (8)

## 4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

| | | |
|---|---|---|
| **Type** | : | static |
| **Species** | : | other: Ceriodaphnia dubia |
| **Exposure period** | : | 48 hour(s) |
| **Unit** | : | mg/l |
| **EC50** | : | = 1.5 measured/nominal |
| **Method** | : | |
| **Year** | : | 1986 |
| **GLP** | : | no data |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |

| | | |
|---|---|---|
| **Test condition** | : | Water Parameters:<br>Temperature (TMP): 25.3 (mean value); Units: C<br>Dissolved O2 (mg/l or % saturation) (DO2): 7.3 (mean value) mg/L<br>pH: 7.86 (mean value) |
| **Test substance** | : | 99.8% purity |
| **Reliability** | : | (2) valid with restrictions<br>Information taken from a peer-reviewed publication. |
| **Flag** | : | Critical study for SIDS endpoint |

28.11.2003 (18)

| | | |
|---|---|---|
| **Type** | : | static |
| **Species** | : | Daphnia magna (Crustacea) |
| **Exposure period** | : | 48 hour(s) |
| **Unit** | : | mg/l |
| **EC50** | : | = 3.9 calculated |
| **Method** | : | |
| **Year** | : | 1972 |
| **GLP** | : | no data |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Source** | : | Epona Asociates, LLC |
| **Test condition** | : | Water Parameters:<br>Temperature : 18 (mean value) C<br>Hardness(mg/l CaCO3): 45.3 (mean value)mg/L CaCO3<br>Alkalinity (mg/l CaCO3): 42.3 (mean value)mg/L CaCO3<br>Dissolved O2 (mg/l or % saturation) : 9 (mean value)mg/L<br>pH : 7.74 (mean value) |
| **Reliability** | : | (2) valid with restrictions<br>Information taken from a peer-reviewed publication. |

28.11.2003 (5)

### 4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

| | | |
|---|---|---|
| **Species** | : | Chlorella vulgaris (Algae) |
| **Endpoint** | : | other: popu;ation growth |
| **Exposure period** | : | |
| **Unit** | : | mg/l |
| **Method** | : | |
| **Year** | : | 2000 |
| **GLP** | : | |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Result** | : | Effect = .225 mg/L |
| **Source** | : | BASF AG Ludwigshafen as cited in ECB IUCLID (2000) |
| **Test condition** | : | 4 months; room–temperature; pH 3.4; highest concentration tolerated: 0.002 g AlCl3 (0.05% w/v) |
| **Reliability** | : | (4) not assignable<br>Original study not reviewed. |

04.12.2003

## 5.1.1 ACUTE ORAL TOXICITY

| | | |
|---|---|---|
| **Type** | : | LD50 |
| **Value** | : | = 370 mg/kg bw |
| **Species** | : | rat |
| **Strain** | : | Sprague-Dawley |
| **Sex** | : | |
| **Number of animals** | : | |
| **Vehicle** | : | |
| **Doses** | : | |
| **Method** | : | |
| **Year** | : | 1987 |
| **GLP** | : | no data |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Source** | : | Epona Asociates, LLC |
| **Reliability** | : | (2) valid with restrictions<br>Information taken from a peer-reviewed publication. |
| **Flag** | : | Critical study for SIDS endpoint |

28.11.2003 (1) (15)

| | | |
|---|---|---|
| **Type** | : | LD50 |
| **Value** | : | = 222 mg/kg bw |
| **Species** | : | mouse |
| **Strain** | : | Swiss Webster |
| **Sex** | : | |
| **Number of animals** | : | |
| **Vehicle** | : | |
| **Doses** | : | |
| **Method** | : | |
| **Year** | : | 1987 |
| **GLP** | : | no data |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Source** | : | Epona Asociates, LLC |
| **Reliability** | : | (2) valid with restrictions<br>Information taken from a peer-reviewed publication. |

28.11.2003 (1) (15)

| | | |
|---|---|---|
| **Type** | : | LD50 |
| **Value** | : | = 770 mg/kg bw |
| **Species** | : | mouse |
| **Strain** | : | other: Dobra Voda |
| **Sex** | : | male |
| **Number of animals** | : | |
| **Vehicle** | : | |
| **Doses** | : | |
| **Method** | : | |
| **Year** | : | 1966 |
| **GLP** | : | no data |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Source** | : | Epona Asociates, LLC |
| **Reliability** | : | (2) valid with restrictions<br>Information taken from a peer-reviewed publication. |

28.11.2003 (1) (25)

### 5.1.2 ACUTE INHALATION TOXICITY

### 5.1.3 ACUTE DERMAL TOXICITY

### 5.1.4 ACUTE TOXICITY, OTHER ROUTES

### 5.4 REPEATED DOSE TOXICITY

| | | |
|---|---|---|
| **Type** | : | Sub-acute |
| **Species** | : | mouse |
| **Sex** | : | female |
| **Strain** | : | Swiss Webster |
| **Route of admin.** | : | oral feed |
| **Exposure period** | : | other: 5 or 7 weeks |
| **Frequency of treatm.** | : | |
| **Post exposure period** | : | |
| **Doses** | : | |
| **Control group** | : | |
| **NOAEL** | : | = 195 mg/kg bw |
| **Method** | : | |
| **Year** | : | 1993 |
| **GLP** | : | no data |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Remark** | : | Approximate feed concentrations of 250 and 350 ppm aluminum (ATSDR, 1999) |
| **Result** | : | Mice that ingested doses higher than 130 mg Al/kg/day as aluminum chloride for 49 days, and were tested using a standardized neurotoxicity screening battery, also showed decreased motor activity, as well as decreased grip strength and startle responsiveness. Signs of neurotoxicity but no change in hematocrit levels, no liver changes at 195 mg/kg/day. No body weight chnages at 260 mg/kg/day. |
| **Source** | : | Epona Asociates, LLC |
| **Test condition** | : | Adult mice consumed aluminum chloride for 5-7 weeks in a diet that also contained 3.5% sodium citrate. |
| **Reliability** | : | (2) valid with restrictions<br>Information taken from a peer-reviewed publication. |

28.11.2003 (1) (26)

| | | |
|---|---|---|
| **Type** | : | Sub-chronic |
| **Species** | : | mouse |
| **Sex** | : | male/female |
| **Strain** | : | other: Dobra Voda |
| **Route of admin.** | : | other: drinking water and base diet |
| **Exposure period** | : | up to 390 days |
| **Frequency of treatm.** | : | |
| **Post exposure period** | : | |
| **Doses** | : | 19.3 or 49 mg/kg/day |
| **Control group** | : | yes |
| **Method** | : | |
| **Year** | : | 1966 |
| **GLP** | : | no |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Result** | : | No change in lung histology and no hepatatic effects when exposed to 19.3 |

mg/kg/day for 390 days.
No effects on body weight at any dose or exposure time. No hematological effects, no histological changes in the femurs of male and female Dobra Voda
mice given 49 mg Al/kg/day as aluminum chloride in drinking water for 180 or 390 days (ATSDR, 1999). No renal effects in male or female animals given 49 mg/kg/day for 180 days or 19.3 mg/kg/day for 390 days.
No organ weight or histological changes in the spleen or thymus and the body weights of male and female Dobra Voda mice were similar to controls following
exposure to 49 mg Al/kg/day as aluminum chloride in drinking water and base diet for 180 or 390 days (ATSDR, 1999)

**Reliability** : (2) valid with restrictions
Information taken from a peer-reviewed publication.

28.11.2003 (1) (25)

28.11.2003

## 5.5 GENETIC TOXICITY 'IN VITRO'

**Type** : Salmonella typhimurium reverse mutation assay
**System of testing** : TA102
**Test concentration** : 0.3, 3 ppm (0.3, 3 mg/l)
**Cycotoxic concentr.** :
**Metabolic activation** :
**Result** : negative
**Method** : other: according to Ames, B.N. et al.: Mutat. Res. 31, 347–164
**Year** : 1985
**GLP** : no data
**Test substance** : no data

**Remark** : Preincubation test with solutions containing 0.3 and 3.0 ppmof the test substance.
**Source** : BASF AG Ludwigshafen as cited in ECB IUCLID (2000) Epona Asociates, LLC
**Reliability** : (2) valid with restrictions
**Flag** : Critical study for SIDS endpoint
04.12.2003 (1) (2) (17)

**Type** : other: Rec Assay
**System of testing** : Bacillus subtilus
**Test concentration** :
**Cycotoxic concentr.** :
**Metabolic activation** :
**Result** : negative
**Method** :
**Year** : 1980
**GLP** : no data
**Test substance** : no data

**Source** : Epona Asociates, LLC
**Reliability** : (2) valid with restrictions
28.11.2003 (1) (14)

**Type** : other: Thymidine incorporation
**System of testing** : rat osteoblasts
**Test concentration** :
**Cycotoxic concentr.** :
**Metabolic activation** :

| | | |
|---|---|---|
| **Result** | : | |
| **Method** | : | |
| **Year** | : | 1989 |
| **GLP** | : | no data |
| **Test substance** | : | |
| **Remark** | : | "aluminum may impede cell cycle progression. Generalizations to normal, untransformed cells, however, cannot be made." (ATSDR, 1999) |
| **Source** | : | Epona Asociates, LLC |
| **Reliability** | : | (2) valid with restrictions |

28.11.2003 (1) (6)

| | | |
|---|---|---|
| **Type** | : | Mammalian cell gene mutation assay |
| **System of testing** | : | Syrian hamster embryo cells |
| **Test concentration** | : | |
| **Cycotoxic concentr.** | : | |
| **Metabolic activation** | : | |
| **Result** | : | negative |
| **Method** | : | |
| **Year** | : | 1979 |
| **GLP** | : | no data |
| **Test substance** | : | no data |
| **Source** | : | Epona Asociates, LLC |
| **Reliability** | : | (2) valid with restrictions<br>Information taken from a peer-reviewed publication. |

28.11.2003 (1) (10)

| | | |
|---|---|---|
| **Type** | : | other: DNA cross-linking |
| **System of testing** | : | Rat ascites hepatoma cells |
| **Test concentration** | : | 500 umol/l |
| **Cycotoxic concentr.** | : | |
| **Metabolic activation** | : | |
| **Result** | : | positive |
| **Method** | : | |
| **Year** | : | 1986 |
| **GLP** | : | no data |
| **Test substance** | : | no data |
| **Remark** | : | "Cross-linking agents frequently produce clastogenic effects due, presumably, to conformational distortions that prohibit proper DNA replication." (ATSDR, 1999) |
| **Source** | : | Epona Asociates, LLC |
| **Reliability** | : | (2) valid with restrictions<br>Information taken from a peer-reviewed publication. |

28.11.2003 (1) (29)

| | | |
|---|---|---|
| **Type** | : | Ames test |
| **System of testing** | : | Salmonella typhimurium TA1537 TA2637 TA98 TA100 TA102 |
| **Test concentration** | : | |
| **Cycotoxic concentr.** | : | |
| **Metabolic activation** | : | |
| **Result** | : | negative |
| **Method** | : | |
| **Year** | : | 1987 |
| **GLP** | : | no data |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Source** | : | BASF AG Ludwigshafen as cited in ECB IUCLID (2000) |
| **Reliability** | : | (4) not assignable |

04.12.2003 (24)

| | | |
|---|---|---|
| **Type** | : | Mouse lymphoma assay |
| **System of testing** | : | L5178Y TK+/– Mouse Lymphoma cells |
| **Test concentration** | : | 570, 580, 590, 600, 620, 625 ug/ml |
| **Cycotoxic concentr.** | : | |
| **Metabolic activation** | : | with and without |
| **Result** | : | negative |
| **Method** | : | other: according to Clive, D. et al.: Mutat. Res. 59, 61–108 |
| **Year** | : | 1979 |
| **GLP** | : | no data |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Remark** | : | forward mutation assay with and without metabolic activationwith S9–mix prepared from liver homogenate of Aroclor pretreated Sprague–Dawley rats; the mutation frequency remained constant at ca. 2–fold |
| **Source** | : | BASF AG Ludwigshafen as cited in ECB IUCLID (2000) |
| **Test substance** | : | aluminium chloride; according to the authors, the compound was of certified ACS grade |
| **Reliability** | : | (4) not assignable<br>Original study not reviewed. |

04.12.2003 (22) (23)

## 5.6 GENETIC TOXICITY 'IN VIVO'

| | | |
|---|---|---|
| **Type** | : | Micronucleus assay |
| **Species** | : | mouse |
| **Sex** | : | |
| **Strain** | : | |
| **Route of admin.** | : | i.p. |
| **Exposure period** | : | bone marrow cells were fixed at times up to 72 h |
| **Doses** | : | .01, .05 or .1 molar aluminum chloride |
| **Result** | : | positive |
| **Method** | : | |
| **Year** | : | 1972 |
| **GLP** | : | no data |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Result** | : | "There was a significant increase in chromatid-type aberrations over the controls, and these occurred in a nonrandom distribution over the chromosome complement. No dose-response relationship could be demonstrated, although the highest dose of aluminum chloride did produce the greatest number of aberrations." (ATSDR, 1999)<br>The effect was qualitatively more or less the same at different intervals as well as at different concentrations in the form of erosion, stickiness, etc. as general and subchromatid, chromatid and chromosome breaks, ranslocations, gaps and constrictions in the individual chromosomes. |
| **Source** | : | BASF AG Ludwigshafen as cited in ECB IUCLID (2000)<br>Epona Asociates, LLC |
| **Test condition** | : | Mice were injected intraperitoneally with 0.01, 0.05, or 0.1 molar aluminum chloride, and bone marrow cells were examined for chromosomal aberrations. |
| **Reliability** | : | (2) valid with restrictions |
| **Flag** | : | Critical study for SIDS endpoint |

04.12.2003 (1) (16)

### 5.8.1 TOXICITY TO FERTILITY

| | | |
|---|---|---|
| **Type** | : | Fertility |
| **Species** | : | rat |
| **Sex** | : | |
| **Strain** | : | Sprague-Dawley |
| **Route of admin.** | : | drinking water |
| **Exposure period** | : | up to 90 d prior to breeding |
| **Frequency of treatm.** | : | |
| **Premating exposure period** | | |
| **Male** | : | 90 days |
| **Female** | : | |
| **Duration of test** | : | 160 days |
| **No. of generation studies** | : | |
| **Doses** | : | 0; 5; 50; 500 mg/l (Al–equivalent) = 0; 44.8; 447.6; 4476.0 mg/l (AlCl3) |
| **Control group** | : | yes, concurrent no treatment |
| **Method** | : | |
| **Year** | : | 1979 |
| **GLP** | : | no data |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Remark** | : | AlCl3 was tested as AlCl3 . 6H2O; molecular weight 241 and aluminium equivalent weight of 11%. |
| **Result** | : | No abnormalities in the reproductive capacity of the males measured by histopathologic evaluation, plasma gonadotropin level and serial mating of the males to untreated virgin females over a 70 d posttreatment breeding period. |
| **Source** | : | BASF AG Ludwigshafen as cited in ECB IUCLID (2000) |
| **Reliability** | : | (4) not assignable<br>Original study not reviewed. |

04.12.2003 (11)

| | | |
|---|---|---|
| **Type** | : | other: three generation |
| **Species** | : | mouse |
| **Sex** | : | |
| **Strain** | : | Swiss Webster |
| **Route of admin.** | : | other: drinking water and base diet |
| **Exposure period** | : | 180 - 390 d (weanlings were treated from 4.week of age like parents)390 days |
| **Frequency of treatm.** | : | |
| **Premating exposure period** | | |
| **Male** | : | |
| **Female** | : | |
| **Duration of test** | : | |
| **No. of generation studies** | : | 3 |
| **Doses** | : | 0; 19.3 mg/kg/d (doses expressed in terms of Al) |
| **Control group** | : | |
| **Result** | : | no effects on fertility |
| **Method** | : | |
| **Year** | : | 1966 |
| **GLP** | : | no |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Remark** | : | "Aluminum apparently does not affect reproduction. Finally, pharmacokinetic data do not indicate that the reproductive organs are target organs" (ATSDR, 1999) |
| **Result** | : | There were no significant differences in the numbers of |

litters or off–spring between the treated and control mice. Growth was retarded and was dependent on the intake of aluminium, but the effect did not appear in the first generation or in the first litter. The subsequent litters manifested a very marked growth retardation, as did those of the third generation. An analysis of variance established that, under the conditions of our experiment, weight variations could be accounted for by aluminium uptake ($P < 0.001$). The differences in the course of weight plots for successive generations and litters were also statistically significant ($P < 0.01$).
The erythrocyte counts and haemoglobin levels in the first and last generations did not differ significantly from those in the controls; and no pathological changes could be found in the tissues examined.

**Source** : BASF AG Ludwigshafen as cited in ECB IUCLID (2000)
Epona Asociates, LLC

**Reliability** : (2) valid with restrictions

**Flag** : Critical study for SIDS endpoint

04.12.2003 (1) (25)

### 5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

| | | |
|---|---|---|
| **Species** | : | rat |
| **Sex** | : | female |
| **Strain** | : | other: THA |
| **Route of admin.** | : | gavage |
| **Exposure period** | : | on day 15 of pregnancy |
| **Frequency of treatm.** | : | single dose |
| **Duration of test** | : | until 10 weeks post parturition |
| **Doses** | : | 900, 1800 mg/kg |
| **Control group** | : | yes, concurrent no treatment |
| **Method** | : | |
| **Year** | : | |
| **GLP** | : | no data |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |

**Remark** : According to the authors, the doses applied in this study corresponded with ca. 1/4 and 1/2 of the acute oral LD50 of the test substance for adult rats.

**Result** : The effects of prenatal aluminium treatment on development and behaviour were studied. Four and three pregnant rats of the 22nd generation of the THA strain were administered the test substance dissolved in saline at doses of 900 and 1800 mg/kg, respectively; another 3 rats were given saline (control). The day of parturition was designated as postnatal day 0. Body weights of the litters were recorded on postnatal days 1, 7, 14, 21, and 28. Pups were weaned at postnatal day 21. Twenty offsprings (10 males and 10 females) each of the dams of each aluminium treated group and 10 males and 18 female offsprings of control dams were selected for behavioural tests (Sidman avoidance test on postnatal days 28 to 38; open field test at 10 weeks post partum).
Statistically significant differences in body weight gain, timing of pinna detachment and eye opening, andappearances of auditory startle were observed between the aluminium treated offspring and controls. Behavioural tests revealed slower learning acquisition in the treated groups.The longer latency and more rearings in the open field test

wereobserved in the female pups of high dose group dams. According to the authors, these results suggested thatsingledose of the test substance during prenatal period affected both the development and behaviour of the offspringin rats.

**Source** : BASF AG Ludwigshafen as cited in ECB IUCLID (2000)
**Test substance** : aluminium chloride; purity >98%
**Reliability** : (4) not assignable
Original study not reviewed.

04.12.2003 (21)

**Species** : rat
**Sex** : female
**Strain** : Sprague-Dawley
**Route of admin.** : oral feed
**Exposure period** : Gestation day 6, 9, 12, 15 and 18
**Frequency of treatm.** : continuously in the diet on treatment days
**Duration of test** : 20 days
**Doses** : 500, 1000 ppm in the diet (ca. 45, 91 mg/kg/d, respectively)
**Control group** :
**NOAEL maternal tox.** : = 110 - mg/kg bw
**Method** :
**Year** : 1979
**GLP** : no data
**Test substance** : as prescribed by 1.1 - 1.4

**Remark** : "The 110 mg Al/kg/day dose is not a definite NOAEL because the intermittent daily exposure schedule could have missed a critical developmental time for inducing effects. Concurrent administration of parathyroid hormone by subcutaneous injection, which increased tissue levels of aluminum by presumably enhancing its absorption, increased the percentage of resorbed or dead fetuses." (ATSDR, 1999)
Comment: Normal food contained 119 ppm Al

**Result** : "Rats that ingested up to 110 mg Al/kg/day in feed that contained added aluminum chloride on Gd 6, 9, 12, 15, and 18 did not experience maternal toxicity, embryo/fetal toxicity, teratogenicity, fetal growth retardation, or significantly increased fetal whole carcass concentrations of aluminum " (ATSDR, 1999)
Resorption rate was increased following 1000 ppm Al and Parathyroid Hormone (PTH) – subcutaneous injections of 68 units/kg on gestational days 6, 9, 12, 15, and 18 – suggesting that this metal and hormone may be embryotoxic when administered throughout organogenesis and late fetal development (day 6–19). Neither PTH nor 1000 ppm Al alone had any effect on mortality and the apparent no–effect dose level for embryotoxicity after combined treatment is 500 ppm Al and PTH.
**Source** : BASF AG Ludwigshafen as cited in ECB IUCLID (2000)
Epona Asociates, LLC
**Reliability** : (2) valid with restrictions
Information taken from a peer-reviewed publication.
**Flag** : Critical study for SIDS endpoint
04.12.2003 (1) (20)

**Species** : rat
**Sex** :
**Strain** : Sprague-Dawley
**Route of admin.** : oral feed
**Exposure period** : from day 6 of gestation through day 19

| | | |
|---|---|---|
| **Frequency of treatm.** | : | continuously in the diet |
| **Duration of test** | : | 20 days |
| **Doses** | : | 0.1 % in the diet (ca. 91 mg/kg/d) |
| **Control group** | : | no data specified |
| **Remark** | : | Maternal tox.: No effect reported |
| **Result** | : | No significant effect on dam body weight gain, fetal weight or length, resorption rate or incidence of soft tissue or skeletal anormalies. |
| **Source** | : | BASF AG Ludwigshafen as cited in ECB IUCLID (2000) |
| **Reliability** | : | (4) not assignable<br>Original study not reviewed. |

04.12.2003 (19)

| | | |
|---|---|---|
| **Species** | : | rat |
| **Sex** | : | female |
| **Strain** | : | other: Holtzmann |
| **Route of admin.** | : | i.p. |
| **Exposure period** | : | days 9-13 or 14-18 of gestation |
| **Frequency of treatm.** | : | 5 times |
| **Duration of test** | : | 20 days |
| **Doses** | : | 0; 75; 100; 200 mg/kg (AlCl3 crystals solved in sterile dist. water) |
| **Control group** | : | yes, concurrent no treatment |
| **Remark** | : | Maternal tox.:<br>– Dose dependent death in 100– and 200 mg/kg group;<br>– Stat. sign. differences in maternal weight gain at dose level 75 and 100 (treated on days 14–18 of ge–station).<br>– In many cases maternal liver was severely damaged (perihepatic granulomas, signs of centrilobular ne–crosis). |
| **Result** | : | Offsprings treated with AlCl3 showed sign growth retardation as well as skeletal defects; incidence of fetal death and resorption was significantly increased.<br>75 mg/kg (day 14–18 of gestation): no malformation<br>There was no clear dose–response relationship respect to mean weight and length of fetuses.<br>100 mg/kg (day 14–18 of gestation): Three fetuses (from 2 litters) had abnormal digits.<br>7 fetuses (from 4 litters) had wavy ribs – in cases ribs were missing.<br>A large number of fetuses showed poor ossification (cranid bones, lower part of vertebral column, bones of limbs).<br>200 mg/kg: High incidence of dead offspring |
| **Source** | : | BASF AG Ludwigshafen as cited in ECB IUCLID (2000) |
| **Reliability** | : | (4) not assignable<br>Original study not reviewed. |

04.12.2003 (4) (13)

(1) Agency for Toxic Substances and Disease Registry [ATSDR] 1999, Toxicological Profile for Aluminum.

(2) Ahn, H.–W. and Jeffery, E.H.: J. Toxicol. Environ. Health 41, 357–368 (1994)b as cited in ECB IUCLID (2000)

(3) BASF AG, Sicherheitsdatenblatt ALUMINIUMCHLORID wasserfrei gebrochen (2/88); as cited in the 2000 ECB IUCLID for aluminum chloride

(4) Benett R.W. et al.: Anat.Anz. 138, 365–378, (1975) as cited in ECB IUCLID (2000)

(5) Biesinger, K.E. and G.M. Christensen (1972) Effects of Various Metals on Survival, Growth, Reproduction, and Metabolism of Daphnia magna. Canada. Fisheries Research Board. Journal, 29(12): 1691-1700; 1972 ISSN: 0008-2686 CIS Record ID.: AQ-0017000

(6) Blair HC, Finch JL, Avioli R, et al. 1989. Micromolar aluminum levels reduce 3H-thymidine incorporation by cell line UMR 106-01. Kidney Int 35:1119-l 125.

(8) Call, DJ, LT Brooke, CA Lindberg, TP MArkee, DJ MaCauley, and SH Poirier (1984) Toxicity of Aluminum to Freshwater Organisms in Water of pH 6.5-8.5. Tech Rep Project No. 549-238-RT-WRD, Center for Lake Superior Environmental Studies, University of Wisconsin, Superior, WI. /November 27, 1984 Memo to C Stephan, USEPA, Duluth, MN:46 p (Author Communication Used).

(9) Dave, G (1985) The Influence of pH on the Toxicity of Alumnium, Cadmium, and Iron to Eggs and Larvae of the Zebrafish, Brachydanio rerio. Ecoxtoxicol Environ Saf 10(2):253-267.

(10) DiPaolo JA, Casto BC. 1979. Quantitative studies of in vitro morphological transformation of Syrian hamster cells by inorganic metal salts. Cancer Res 39:1008-1013.

(11) Dixon R.L. et al.: Environ. Health Persp. 30, 53–68, (1979) as cited in ECB IUCLID (2000)

(12) ECB (2000) IUCLID for Aluminum Chloride

(13) Elinder C.–G. and Sjoegren B. in: Friberg L.(Ed.) et al.: Handbook on the Toxicology Metals, 2nd. Ed., 1–25, Elsevier, (1986) as cited in ECB IUCLID (2000)

(14) Kanematsu N, Hara M, Kada T. 1980. Ret assay and mutagenicity studies on metal compounds. Mutat Res 77:109-116.

(15) Llobet JM, Domingo JL, Gomez M, et al. 1987. Acute toxicity studies of aluminum compounds: Antidotal efficacy of several chelating agents. Pharmacol Toxico1 60:280-283.Liobet et al (1987)

(16) Manna GK, Das RK. 1972. Chromosome aberrations in mice induced by aluminum chloride. Nucleus 15:180-186.

(17) Marzin DR, Phi HV. 1985. Study of the mutagenicity of metal derivatives with salmonella typhimurium TA102m Mutat Res 155:49-52.

(18) McCauley, D.J., L.T. BROOKE, D.J. CALL and C.A. LINDBERG (1986) Acute and Chronic Toxicity of Aluminum to Ceriodaphnia dubia at Various pH's. Center for Lake Superior Environmental Studies, University of Wisconsin, Superior, WI: 15; 1986 CIS Record ID.: AQ-0113175

(19) Mccormack K.M. et al.: Teratology 17, 50 A, (1978) as cited in ECB IUCLID (2000)

(20) McCormack KM, Ottosen LD, Sanger VL, et al. 1979. Effect of prenatal administration of aluminum
and parathyroid hormone on fetal development in the rat (40493). Proc Sot Exp Biol Med 161:74-77.

(21) Misawa, T. and Shigeta, S.: J. Toxicol. Sci. 18, 43–48
(1993) as cited in ECB IUCLID (2000)

(22) Oberly T.J. and Piper C.E.: Environ. Mutag. 2, 281 (1980);
abstract as cited in ECB IUCLID (2000)

(23) Oberly T.J. et al.: J. Toxicol. Environ. Health 9, 367–376
(1982) as cited in ECB IUCLID (2000)

(24) Ogawa H.I. et al.: Jpn.J.Genet. 62, 159–162, (1987)

(25) Ondreicka R, Ginter E, Kortus J. 1966. Chronic toxicity of aluminum in rats and mice and its effects
on phosphorus metabolism Br J Ind Med 23:305-312.

(26) Oteiza PI, Keen CL, Han B, et al. 1993. Aluminum accumulation and neurotoxicity in Swiss-mice after long-term dietary exposure to aluminum and citrate. Metabolism 42:1296-1300.

(27) Wallen, IE, WC Greer and R Lasater (1957) Toxicity to Gambusia affinus of Certain Pure Chemcials in Turbid Water. Sewage Ind Wastes 29(6):695-711.

(28) Weast, R.C. (1969) Chemical Rubber Company Handbook of Chemistry and Physics. 50th Ed, CRC Press, Inc. Cleveland, Ohio, 1969

(29) Wedrychowski A, Schmidt WN, Hnilica LS. 1986. The in-vivo cross-linking of proteins and DNA by
heavy metals. J Biol Chem 261:3370.

# IUCLID

# Data Set

| | | |
|---|---|---|
| **Existing Chemical** | : | ID: 300-92-5 |
| **CAS No.** | : | 300-92-5 |
| **EINECS Name** | : | hydroxyaluminium distearate |
| **EC No.** | : | 206-101-8 |
| **Molecular Formula** | : | C36H71AlO5 |

**Producer related part**

| | | |
|---|---|---|
| **Company** | : | Epona Associates, LLC |
| **Creation date** | : | 05.12.2003 |

**Substance related part**

| | | |
|---|---|---|
| **Company** | : | Epona Associates, LLC |
| **Creation date** | : | 05.12.2003 |
| **Status** | : | |
| **Memo** | : | SOCMA MCC |
| **Printing date** | : | 25.01.2007 |
| **Revision date** | : | |
| **Date of last update** | : | 25.01.2007 |
| **Number of pages** | : | 26 |
| **Chapter (profile)** | : | Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10 |
| **Reliability (profile)** | : | Reliability: without reliability, 1, 2, 3, 4 |
| **Flags (profile)** | : | Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS |

### 1.0.1 APPLICANT AND COMPANY INFORMATION

### 1.0.2 LOCATION OF PRODUCTION SITE, IMPORTER OR FORMULATOR

### 1.0.3 IDENTITY OF RECIPIENTS

### 1.0.4 DETAILS ON CATEGORY/TEMPLATE

### 1.1.0 SUBSTANCE IDENTIFICATION

### 1.1.1 GENERAL SUBSTANCE INFORMATION

| | | |
|---|---|---|
| **Purity type** | **:** | |
| **Substance type** | **:** | organic |
| **Physical status** | **:** | solid |
| **Purity** | **:** | |
| **Colour** | **:** | white |
| **Odour** | **:** | |
| **Reliability** | **:** | (2) valid with restrictions<br>Information taken from a peer-reviewed publication. |

18.10.2006 (5)

### 1.1.2 SPECTRA

### 1.2 SYNONYMS AND TRADENAMES

### 1.3 IMPURITIES

### 1.4 ADDITIVES

### 1.5 TOTAL QUANTITY

### 1.6.1 LABELLING

### 1.6.2 CLASSIFICATION

### 1.6.3 PACKAGING

**1.7 USE PATTERN**

**1.7.1 DETAILED USE PATTERN**

**1.7.2 METHODS OF MANUFACTURE**

**1.8 REGULATORY MEASURES**

**1.8.1 OCCUPATIONAL EXPOSURE LIMIT VALUES**

**1.8.2 ACCEPTABLE RESIDUES LEVELS**

**1.8.3 WATER POLLUTION**

**1.8.4 MAJOR ACCIDENT HAZARDS**

**1.8.5 AIR POLLUTION**

**1.8.6 LISTINGS E.G. CHEMICAL INVENTORIES**

**1.9.1 DEGRADATION/TRANSFORMATION PRODUCTS**

**1.9.2 COMPONENTS**

**1.10 SOURCE OF EXPOSURE**

**1.11 ADDITIONAL REMARKS**

**1.12 LAST LITERATURE SEARCH**

**1.13 REVIEWS**

### 2.1 MELTING POINT

| | | |
|---|---|---|
| **Value** | : | = 145 °C |
| **Sublimation** | : | |
| **Method** | : | |
| **Year** | : | 1987 |
| **GLP** | : | no data |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Reliability** | : | (2) valid with restrictions<br>Information taken from a peer-reviewed publication. |
| **Flag** | : | Critical study for SIDS endpoint |

05.12.2003 (5)

### 2.2 BOILING POINT

| | | |
|---|---|---|
| **Decomposition** | : | yes |
| **Method** | : | |
| **Year** | : | 2003 |
| **GLP** | : | no |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Remark** | : | The boiling points of the dissociation products are: 190 deg C (aluminum chloride) and 69-70 deg C (Stearic acid).<br>This endpoint is not applicable due to the physical state the substance. The substance will decompose upon heating. |
| **Reliability** | : | (2) valid with restrictions |
| **Flag** | : | Critical study for SIDS endpoint |

18.10.2006 (2)

### 2.3 DENSITY

#### 2.3.1 GRANULOMETRY

### 2.4 VAPOUR PRESSURE

| | | |
|---|---|---|
| **Decomposition** | : | |
| **Method** | : | |
| **Year** | : | 2003 |
| **GLP** | : | no |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Remark** | : | The estimated vapor pressure is 4E-17 mm Hg EPI SUMMARY (v3.11)<br>The vapor pressures of the dissociation products are: 1.38 @ 100 deg C (aluminum chloride) and 1.33 @ 174 deg C (Stearic acid).<br>This endpoint is not applicable due to the physical state the substance. |
| **Reliability** | : | (2) valid with restrictions |

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## 2.5 PARTITION COEFFICIENT

| | | |
|---|---|---|
| **Partition coefficient** | : | octanol-water |
| **Log pow** | : | at °C |
| **pH value** | : | |
| **Method** | : | |
| **Year** | : | 2003 |
| **GLP** | : | no |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Remark** | : | Aluminum distearate is not soluble in water.<br>The partition coefficients of the dissociation products are:<br>1.26 (calculated) (aluminum chloride) and 8.42 (Stearic acid). |
| **Reliability** | : | (2) valid with restrictions |

06.12.2003

## 2.6.1 SOLUBILITY IN DIFFERENT MEDIA

| | | |
|---|---|---|
| **Solubility in** | : | Water |
| **Value** | : | at °C |
| **pH value** | : | |
| **concentration** | : | at °C |
| **Temperature effects** | : | |
| **Examine different pol.** | : | |
| **pKa** | : | at 25 °C |
| **Description** | : | not soluble |
| **Stable** | : | |
| **Deg. product** | : | |
| **Method** | : | |
| **Year** | : | 2003 |
| **GLP** | : | |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Remark** | : | Water Solubility Estimate from Log Kow (WSKOW v1.41)<br>Water Solubility at 25 deg C (mg/L): 1.776e-0<br>Aluminum distearate is not soluble in water.<br>The water solubilities of the dissociation products are:<br>450 @ 20 deg C (aluminum chloride) and .00568 @ 25 deg C (Stearic acid). |
| **Reliability** | : | (2) valid with restrictions |

06.12.2003

## 2.6.2 SURFACE TENSION

## 2.7 FLASH POINT

## 2.8 AUTO FLAMMABILITY

## 2.9 FLAMMABILITY

### 2.10 EXPLOSIVE PROPERTIES

### 2.11 OXIDIZING PROPERTIES

### 2.12 DISSOCIATION CONSTANT

| | | |
|---|---|---|
| **Method** | : | |
| **Year** | : | 2003 |
| **GLP** | : | |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Remark** | : | The dissociation constants for 18 related metal carboxylate compounds tested have pKa (pKb) values (pKa1) in the neutral range (5.088 to 8.448). This indicates that in the neutral pH range, significant portions of the metal carboxylates will be dissociated. In addition, at the low pH of the mammalian stomach (pH 1.2) all of the metal carboxylates would be expected to be completely or nearly completely dissociated. This indicates that the absorption and any observed toxicity would be independent for the respective acid and metal when administered orally. The aluminum stearate compounds are expected to behave similarly. |
| **Reliability** | : | (1) valid without restriction |
| 06.12.2003 | | |

### 2.13 VISCOSITY

### 2.14 ADDITIONAL REMARKS

### 3.1.1 PHOTODEGRADATION

| | | |
|---|---|---|
| **Type** | : | air |
| **Light source** | : | |
| **Light spectrum** | : | nm |
| **Relative intensity** | : | based on intensity of sunlight |
| **DIRECT PHOTOLYSIS** | | |
| **Halflife t1/2** | : | = .2 day(s) |
| **Degradation** | : | % after |
| **Quantum yield** | : | |
| **INDIRECT PHOTOLYSIS** | | |
| **Sensitizer** | : | |
| **Conc. of sensitizer** | : | |
| **Rate constant** | : | = .000000000043 cm³/(molecule*sec) |
| **Degradation** | : | % after |
| **Deg. product** | : | |
| **Method** | : | other (calculated) |
| **Year** | : | 2003 |
| **GLP** | : | no |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |

**Result** : Atmospheric Oxidation (25 deg C) [AopWin v1.91]:
Hydroxyl Radicals Reaction:
OVERALL OH Rate Constant = 43.0498 E-12 cm3/molecule-sec
Half-Life = 0.248 Days (12-hr day; 1.5E6 OH/cm3)
Half-Life = 2.981 Hrs
Ozone Reaction:
No Ozone Reaction Estimation

**Reliability** : (2) valid with restrictions
**Flag** : Critical study for SIDS endpoint
18.10.2006 (1)

### 3.1.2 STABILITY IN WATER

| | | |
|---|---|---|
| **Deg. product** | : | |
| **Method** | : | |
| **Year** | : | 2003 |
| **GLP** | : | no |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |

**Remark** : Aluminum distearate is not soluble in water.
The hydrolysis data for the dissociation products is:
"unstable" (aluminum chloride) and not avaiable due to low water solubility (stearic acid)

**Reliability** : (2) valid with restrictions
**Flag** : Critical study for SIDS endpoint
18.10.2006

### 3.1.3 STABILITY IN SOIL

### 3.2.1 MONITORING DATA

### 3.2.2 FIELD STUDIES

### 3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

| | | |
|---|---|---|
| **Type** | : | fugacity model level III |
| **Media** | : | |
| **Air** | : | % (Fugacity Model Level I) |
| **Water** | : | % (Fugacity Model Level I) |
| **Soil** | : | % (Fugacity Model Level I) |
| **Biota** | : | % (Fugacity Model Level II/III) |
| **Soil** | : | % (Fugacity Model Level II/III) |
| **Method** | : | other: modeling |
| **Year** | : | 2003 |
| **Result** | : | Level III Fugacity Model:<br>Mass Amount (percent) Half-Life (hr) Emissions (kg/hr)<br>Air 0.126 5.96 1000<br>Water 3.35 900 1000<br>Soil 30 900 1000<br>Sediment 66.5 3.6e+003 0<br>Persistence Time: 1.69e+003 |
| **Reliability** | : | (2) valid with restrictions |
| **Flag** | : | Critical study for SIDS endpoint |

18.10.2006

### 3.3.2 DISTRIBUTION

### 3.4 MODE OF DEGRADATION IN ACTUAL USE

### 3.5 BIODEGRADATION

| | | |
|---|---|---|
| **Deg. product** | : | |
| **Method** | : | |
| **Year** | : | 2003 |
| **GLP** | : | no |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Remark** | : | Aluminum distearate is not soluble in water.<br>The biodegradation of the dissociation products are: not applicable - unstable in water (aluminum chloride) and readily biodegradable (Stearic acid). |
| **Result** | : | Type:aerobic<br>Inoculum:activated sludge<br>Degradation:= 77 - (±) % after 28 day(s)<br>Result: readily biodegradable<br>Kinetic of testsubst.:<br>10 day(s) = 65 - %<br>14 day(s) = 69 - %<br>28 day(s) = 77 - %<br><br>Method: other: BOD test<br>Year:1983 |

GLP:no data
Test substance: stearic acid

Remark: Results are an average of 11 participating laboratories.
Result: 65, 69 and 77 % degradation after 10, 14 and 28 days, respectively.
Reference: King, E.F.; Painter, H.A. (1983) RING-TEST PROGRAM 1981-1982. ASSESSMENT OF BIODEGRADABILITY OF CHEMICALS IN WATER BY MANOMETRIC RESPIROMETRY. COMM. EUR.
COMMUNITIES, EUR 8631. 31 PP, 1983 CIS Record ID.: BD-0000218 publication.

**Reliability** : (2) valid with restrictions
**Flag** : Critical study for SIDS endpoint
18.10.2006

## 3.6 BOD5, COD OR BOD5/COD RATIO

## 3.7 BIOACCUMULATION

## 3.8 ADDITIONAL REMARKS

## 4.1 ACUTE/PROLONGED TOXICITY TO FISH

**Method** :
**Year** : 2003
**GLP** :
**Test substance** : other TS

**Remark** : Aluminum distearate is not soluble in water, and is expected to readily dissociate to Aluminum and Stearic acid.
Species:Oncorhynchus mykiss (Fish, fresh water)
Exposure period 96 hour(s)
Unit: mg/l
LC50: = 8.6
Test Substance: Aluminum chloride
Reference: Call, DJ, LT Brooke, CA Lindberg, TP MArkee, DJ MaCauley, and SH Poirier (1984) Toxicity of Aluminum to Freshwater Organisms in Water of pH 6.5-8.5. Tech Rep Project No. 549-238-RT-WRD, Center for Lake Superior Environmental Studies, University of Wisconsin, Superior, WI. /November 27, 1984 Memo to C Stephan, USEPA, Duluth, MN:46 p (Author Communication Used).
Type:static
Species:Oncorhynchus kisutch (Fish, fresh water, marine)
Exposure period:96 hour(s)
Unit: µg/l
LC50: = 12000 - measured/nominal
Method:
Year: 1977
GLP: no data
Test substance: Stearic acid

Test substance: "pure"
Reliability: (2) valid with restrictions
Flag: Critical study for SIDS endpoint
Reference: SIDS Leach, J.M. and A.N. Thakore (1977) Compounds Toxic to Fish Pulp Mill Waste Streams Progress in Water Technology, 9: 787-798 CIS Record ID.: AQ-0132049

**Reliability** : (2) valid with restrictions
**Flag** : Critical study for SIDS endpoint
18.10.2006

## 4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

**Method** :
**Year** : 2003
**GLP** :
**Test substance** : other TS

**Remark** : Acute toxicity to aquatic invertebrates was not located for stearic acid.
Aluminum distearate is not soluble in water, and is expected to readily dissociate to Aluminum and Stearic acid.
Type:static
Species other: Ceriodaphnia dubia
Exposure period : 48 hour(s)
Unit: mg/l
EC50: = 1.5 - measured/nominal

Method:
Year: 1986
GLP: no data
Test substance: as prescribed by 1.1 - 1.4

Test condition: Water Parameters:
Temperature (TMP): 25.3 (mean value); Units: C
Dissolved O2 (mg/l or % saturation) (DO2): 7.3 (mean value) mg/L
pH: 7.86 (mean value)

Test substance: Aluminum chloride, 99.8% purity
Reliability: (2) valid with restrictions
Information taken from a peer-reviewed publication.
Flag: Critical study for SIDS endpoint
Reference: McCauley, D.J., L.T. BROOKE, D.J. CALL and C.A. LINDBERG (1986) Acute and Chronic Toxicity of Aluminum to Ceriodaphnia dubia at Various pH's. Center for Lake Superior Environmental Studies, University of Wisconsin, Superior, WI: 15; 1986 CIS Record ID.: AQ-0113175

**Reliability** : (2) valid with restrictions
**Flag** : Critical study for SIDS endpoint
18.10.2006

## 4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

**Method** :
**Year** : 2003
**GLP** : no
**Test substance** : other TS

**Remark** : Acute toxicity to aquatic invertebrates or aquatic plants was not located for stearic acid or aluminum chloride. Aluminum distearate is not soluble in water, and is expected to readily dissociate to Aluminum and Stearic acid.
**Reliability** : (2) valid with restrictions
18.10.2006

## 4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

### 4.5.1 CHRONIC TOXICITY TO FISH

### 4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

**Species** : Daphnia magna (Crustacea)
**Endpoint** : reproduction rate
**Exposure period** : 21 day(s)
**Unit** : mg/l
**NOEC** : = .0061
**LOEC** : = .02
**EC50** : = .059
**Analytical monitoring** : yes
**Method** : OECD Guide-line 211
**Year** : 2007
**GLP** : yes

**Test substance** : as prescribed by 1.1 - 1.4

**Method** : Also in accordance with Method C.20 of Commission Directive 2001/59/EC (which constitutes Annex V of Council Directive 67/548/EEC).

Based on the results of a preliminary range-finding test, Daphnia magna were exposed (10 relicates of a single daphnid per group) to an aqueous solution of the test material over a range of test concentrations of 0.0021, 0.0061, 0.020, 0.062 and 0.19 mg/L for a period of 21 days. The test solutions were prepared by stirring an excess (100 mg/L) of test material in reconstituted water at approximately 1500 rpm at a temperature of approximately 21 oC for 24 hours prior to removing any undissolved test material by filtration (0.2 um Sartorius Sartopore filter) to give a saturated solution with a nominal concentration of 0.19 mg/L (based on chemical analysis of saturated solutions prepared during the definitive test). The test solutions were renewed 3 times per week. The numbers of live and dead adult Daphnia and young daphnids (live and dead) were determined daily. The Daphnia were fed daily with an algal suspension.

**Result** : The 14- and 21-day EC50 (immobilization) values, based on nominal test concentrations for the parental Daphnia generation (P1) were calculated to be 0.24 and 0.048 mg/L with 95% confidence limits of 0.13 - 1300* mg/L and 0.0028 - 0.31 mg/L, respectively. The upper 95% confidence limit for the 14-day EC50 value should be viewed with caution as the test material is insoluble at this concentration.

The 21-day EC50 (reproduction) value based on nominal test concentrations was calculated to be 0.059 mg/L with 95% confidence limits of 0.031 - 0.15 mg/L.

The 21-day EC50 for immobilization was calculated to be greater than the EC50 for reproduction. This was due to the 20% mortalities observed at the 0.0021 and 0.0061 mg/L test concentrations. These mortalities were considered to be due to handling stress and/or natural causes as these daphnids were observed to produce young prior to mortality. The observed mortalities were shown not to be statistically significant from the control. In addition, although the test material had an effect on mortality of the parental generation, it did not affect the reproduction of the surviving daphnia.

The LOEC was considered to be 0.020 mg/L on the basis that at this test concentration significantly fewer live young per adult ($P<0.05$) were produced when compared to the control.

The NOEC was considered to be 0.0061 mg/L on the basis that at this test concentration there were no significant mortalities (immobilization) observed in the parental generation (P1) compared to the control and that there were no significant differences ($P>=0.05$) between the control and the 0.0061 mg/L test group in terms of numbers of live young produced per adult by Day 21.

Analysis of the fresh media on Days 0, 4, 7, 11 and 14 showed measured concentrations of 81% to 116% of nominal with the exception of the 0.0021 mg/L test concentration on Days 7 and 11 and the 0.0061 mg/L test concentration on Day 14, which showed measured test concentrations of 75%, 171%, and 126% of nominal, respectively.

Analysis of the old media on Days 0, 5, 8, 12, 15, 19 and 21 showed measured concentrations of 83% to 117% of nominal with the exception of the 0.0021 mg/L test concentration on Days 8 and 12 and the 0.0061 mg/L test concentration on Days 8 and 15, which showed measured test concentrations of 73%, 138%, 77% and 128% of nominal, respectively.

Some of the measured concentrations were shown to be outside the 80% to 120% confidence limits. However, these were considered not to affect the outcome or integrity of the test as the overall means for the fresh and old media were 106% and 96%, respectively.

*The upper 95% confidence limit for the 14-day EC50 value should be viewed with caution. No concentration resulted in greater than 50% immobilization at this time point. Therefore, calculation of the upper confidence limit was affected by the lack of data points above 50% immobilization, hence the very wide confidence interval.

**Reliability** : (1) valid without restriction
Guideline study

**Flag** : Critical study for SIDS endpoint

25.01.2007 (4)

### 4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS

### 4.6.2 TOXICITY TO TERRESTRIAL PLANTS

### 4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS

### 4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES

### 4.7 BIOLOGICAL EFFECTS MONITORING

### 4.8 BIOTRANSFORMATION AND KINETICS

### 4.9 ADDITIONAL REMARKS

## 5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

## 5.1.1 ACUTE ORAL TOXICITY

**Method** :
**Year** : 2003
**GLP** :
**Test substance** : other TS: Dissociation products

**Remark** : Aluminum distearate is expected to readily dissociate to Aluminum and Stearic acid.
Type: LD50
Value: = 370 - mg/kg bw
Species: rat
Strain: Sprague-Dawley
Year: 1987
GLP: no data
Test substance: Aluminum chloride
Reliability: (2) valid with restrictions
Information taken from a peer-reviewed publication.
Flag: Critical study for SIDS endpoint
Reference: Agency for Toxic Substances and Disease Registry [ATSDR] 1999, Toxicological Profile for Alumunim; and Llobet JM, Domingo JL, Gomez M, et al. 1987. Acute toxicity studies of aluminum compounds:
Antidotal efficacy of several chelating agents. Pharmacol Toxicol 60:280-283.Liobet et al (1987)
Type: LD50
Value: = 4600 - mg/kg bw
Species: rat
GLP: no data
Test substance: stearic acid
Reliability: (2) valid with restrictions
Information taken from a peer-reviewed publication.
Reference: Clayton, G.D., F.E. Clayton (eds.) Patty's Industrial Hygiene and Toxicology. Volumes 2A, 2B, 2C, 2D, 2E, 2F: Toxicology. 4th ed. New York, NY: John Wiley & Sons Inc., 1993-1994. 3568. Cited in BiblioLine

**Reliability** : (2) valid with restrictions
18.10.2006

## 5.1.2 ACUTE INHALATION TOXICITY

## 5.1.3 ACUTE DERMAL TOXICITY

## 5.1.4 ACUTE TOXICITY, OTHER ROUTES

## 5.2.1 SKIN IRRITATION

### 5.2.2 EYE IRRITATION

### 5.3 SENSITIZATION

### 5.4 REPEATED DOSE TOXICITY

| | | |
|---|---|---|
| **Type** | : | Sub-acute |
| **Species** | : | rat |
| **Sex** | : | male/female |
| **Strain** | : | Sprague-Dawley |
| **Route of admin.** | : | gavage |
| **Exposure period** | : | 7 days |
| **Frequency of treatm.** | : | daily |
| **Post exposure period** | : | none |
| **Doses** | : | 150, 500 and 1000 mg/kg bw/d |
| **Control group** | : | yes, concurrent vehicle |
| **NOAEL** | : | 1000 - mg/kg bw |
| **Method** | : | The test material was administered by gavage to three groups, each of five male and five female Sprague-Dawley Crl:CD® (SD) IGS BR strain rats, for seven consecutive days, at dose levels of 150, 500 and 1000 mg/kg/day. A control group of five males and five females was dosed with vehicle alone (Arachis oil BP). Clinical signs, bodyweight development and food and water consumption were monitored during the study. Organ weight data was evaluated at the end of the study and all animals were subjected to a gross necropsy examination. |
| **Result** | : | Mortality. There were no mortalities throughout the study. Clinical Observations. There were no treatment-related clinical signs of toxicity observed. Bodyweight. There was a reduction in bodyweight gain for females treated with 1000 mg/kg/day between Days 1 and 4 of treatment. Food Consumption. No treatment-related effects were detected. Water Consumption. No treatment-related effects were detected. Organ Weights. No treatment-related effects were detected. Necropsy. No treatment-related macroscopic abnormalities were detected.<br><br>Conclusion. Oral administration of Aluminium Stearate to rats, by gavage, at dose levels of 150, 500 and 1000 mg/kg/day for seven consecutive days resulted in a transient reduction in bodyweight gain for females treated with 1000 mg/kg/day. In the absence clinical signs of toxicity, this transient effect on bodyweight gain was considered not to have a detrimental effect on the health of the animals. The No Observed Adverse Effect Level (NOAEL) was therefore considered to be 1000 mg/kg/day. |
| **Reliability** | : | (2) valid with restrictions |

Provides basic data
**Flag** : Critical study for SIDS endpoint
18.10.2006 (3)

**Method** :
**Year** : 2003
**GLP** :
**Test substance** : other TS: Dissociation products

**Remark** : Aluminum distearate is expected to readily dissociate to Aluminum and Stearic acid.
Type: Sub-acute
Species: mouse
Sex: female
Strain: Swiss Webster
Route of admin.: oral feed
Exposure period: other: 5 or 7 weeks
NOAEL: = 195 - mg/kg bw
Year: 1993
GLP: no data
Test substance: Aluminum chloride

Remark: Approximate feed concentrations of 250 and 350 ppm aluminum (ATSDR, 1999)
Result: Mice that ingested doses higher than 130 mg Al/kg/day as aluminum chloride for 49 days, and were tested using a standardized neurotoxicity screening battery, also showed decreased motor activity, as well as decreased grip strength and startle responsiveness. Signs of neurotoxicity but no change in hematocrit levels, no liver changes at 195 mg/kg/day. No body weight chnages at 260 mg/kg/day.
Test condition: Adult mice consumed aluminum chloride for 5-7 weeks in a diet that also contained 3.5% sodium citrate.
Reliability: (2) valid with restrictions
Information taken from a peer-reviewed publication.
Reference: Agency for Toxic Substances and Disease Registry [ATSDR] 1999, Toxicological Profile for Aluminum; and Oteiza PI, Keen CL, Han B, et al. 1993. Aluminum accumulation and neurotoxicity in Swiss-mice after long-term dietary exposure to aluminum and citrate. Metabolism 42:1296-1300.
Type: Sub-chronic
Species: rat
Route of admin.: oral feed
Exposure period: 24 weeks
Doses: 50g/kg/day
GLP: no data
Test substance: Stearic acid

Result: Rats fed 50 g/kg/day stearic acid for 24 weeks developed reversible lipogranulomas in adipose tissue. No significant pathological lesions were observed in rats fed 3000 ppm stearic acid orally for about 30 weeks, but anorexia, increased mortality, and a greater incidence of pulmonary infection were observed. Stearic acid is one of the least effective fatty acids in producing hyperlipemia, but the most potent in diminishing blood clotting time.
Reliability: (2) valid with restrictions
Information taken from a peer-reviewed publication.
Reference: Clayton, G.D., F.E. Clayton (eds.) Patty's Industrial Hygiene and Toxicology. Volumes 2A, 2B, 2C, 2D, 2E, 2F: Toxicology. 4th ed. New York, NY: John Wiley & Sons

Inc., 1993-1994. 3568. Cited in BiblioLine

**Reliability** : (2) valid with restrictions
**Flag** : Critical study for SIDS endpoint
18.10.2006

## 5.5 GENETIC TOXICITY 'IN VITRO'

**Type** :
**System of testing** :
**Test concentration** :
**Cycotoxic concentr.** :
**Metabolic activation** :
**Result** :
**Method** :
**Year** : 2003
**GLP** :
**Test substance** : other TS: Dissociation products

**Remark** : Aluminum distearate is expected to readily dissociate to Aluminum and Stearic acid.
Genotoxicity data were not located for Stearic Acid.
Multiple studies with bacterial systems indicate aluminum chloride is not a bacterial mutagen. This is one of several studies sumamrized in the Aluminum chloride IUCLID.
Type: Ames test
System of testing: Salmonella typhimurium TA1537 TA2637 TA98 TA100 TA102
Test concentration:
Result: negative
Year: 1987
GLP: no data
Test substance: Aluminum chloride
Source: BASF AG Ludwigshafen as cited in ECB IUCLID (2000)
Reliability: (4) not assignable
Reference: Ogawa H.I. et al.: Jpn.J.Genet. 62, 159-162, (1987)
Multiple studies with in vitro mammalian systems indicate aluminum chloride is not genotoxic. This is one of several studies sumamrized in the Aluminum chloride IUCLID.

Type: Mouse lymphoma assay
System of testing: L5178Y TK+/- Mouse Lymphoma cells
Test concentration: 570, 580, 590, 600, 620, 625 ug/ml
Metabolic activation: with and without
Result: negative
Method: other: according to Clive, D. et al.: Mutat. Res. 59, 61-108
Year: 1979
GLP: no data
Test substance: Aluminum chloride
Remark: forward mutation assay with and without metabolic activationwith S9-mix prepared from liver homogenate of Aroclor pretreated Sprague-Dawley rats; the mutation frequency remained constant at ca. 2-fold
Source: BASF AG Ludwigshafen as cited in ECB IUCLID (2000)
Test substance: aluminium chloride; according to the authors, the compound was of certified ACS grade
Reliability: (4) not assignable
Original study not reviewed.
Reference: Oberly T.J. and Piper C.E.: Environ. Mutag.

2, 281 (1980); abstract as cited in ECB IUCLID (2000); and Oberly T.J. et al.: J. Toxicol. Environ. Health 9, 367-376 (1982) as cited in ECB IUCLID (2000)

**Reliability** : (2) valid with restrictions
**Flag** : Critical study for SIDS endpoint
18.10.2006

## 5.6 GENETIC TOXICITY 'IN VIVO'

**Type** :
**Species** :
**Sex** :
**Strain** :
**Route of admin.** :
**Exposure period** :
**Doses** :
**Result** :
**Method** :
**Year** : 2003
**GLP** :
**Test substance** : other TS: Dissociation products

**Remark** : Aluminum distearate is expected to readily dissociate to Aluminum and Stearic acid.
Genotoxicity data were not located for Stearic Acid.
Type: Micronucleus assay
Species: mouse
Route of admin.: i.p.
Exposure period : bone marrow cells were fixed at times up to 72 h
Doses: .01, .05 or .1 molar aluminum chloride
Result: positive
Year: 1972
GLP: no data
Test substance: Aluminum chloride
Result: "There was a significant increase in chromatid-type aberrations over the controls, and these occurred in a nonrandom distribution over the chromosome complement. No dose-response relationship could be demonstrated, although the highest dose of aluminum chloride did produce the greatest number of aberrations." (ATSDR, 1999)
The effect was qualitatively more or less the same at different intervals as well as at different concentrations in the form of erosion, stickiness, etc. as general and subchromatid, chromatid and chromosome breaks, ranslocations, gaps and constrictions in the individual chromosomes.
Source: BASF AG Ludwigshafen as cited in ECB IUCLID (2000) Epona Asociates, LLC
Test condition: Mice were injected intraperitoneally with 0.01, 0.05, or 0.1 molar aluminum chloride, and bone marrow cells were examined for chromosomal aberrations.
Reliability: (2) valid with restrictions
Flag: Critical study for SIDS endpoints.
Reference: Agency for Toxic Substances and Disease Registry [ATSDR] 1999, Toxicological Profile for Aluminum; and Manna GK, Das RK. 1972. Chromosome aberrations in mice induced by aluminum chloride. Nucleus

15:180-186.
**Reliability** : (2) valid with restrictions
**Flag** : Critical study for SIDS endpoint
18.10.2006

## 5.7 CARCINOGENICITY

## 5.8.1 TOXICITY TO FERTILITY

**Method** :
**Year** : 2003
**GLP** :
**Test substance** : other TS: Dissociation products

**Remark** : Aluminum distearate is expected to readily dissociate to Aluminum and Stearic acid.
Effects on fertilitydata were not located for Stearic Acid.
Type: other: three generation
Species: mouse
Strain: Swiss Webster
Route of admin.: other: drinking water and base diet
Exposure period: 180 - 390 d (weanlings were treated from 4.week of age like parents)390 days
No. of generation studies: 3
Doses: 0; 19.3 mg/kg/d (doses expressed in terms of Al)
Result: no effects on fertility
Year: 1966
GLP: no data
Test substance: Aluminum chloride
Remark: "Aluminum apparently does not affect reproduction. Finally, pharmacokinetic data do not indicate that the reproductive organs are target organs" (ATSDR, 1999)
Result: There were no significant differences in the numbers of litters or off-spring between the treated and control mice. Growth was retarded and was dependent on the intake of aluminium, but the effect did not appear in the first generation or in the first litter. The subsequent litters manifested a very marked growth retardation, as did those of the third generation. An analysis of variance established that, under the conditions of our experiment, weight variations could be accounted for by aluminium uptake ($P < 0.001$). The differences in the course of weight plots for successive generations and litters were also statistically significant ($P < 0.01$).
The erythrocyte counts and haemoglobin levels in the first and last generations did not differ significantly from those in the controls; and no pathological changes could be found in the tissues examined.
Source: BASF AG Ludwigshafen as cited in ECB IUCLID (2000)
Reliability: (2) valid with restrictions
Reference: Agency for Toxic Substances and Disease Registry [ATSDR] 1999, Toxicological Profile for Aluminum;
and Ondreicka R, Ginter E, Kortus J. 1966. Chronic toxicity of aluminum in rats and mice and its effects on phosphorus metabolism Br J Ind Med 23:305-312.
**Reliability** : (2) valid with restrictions
**Flag** : Critical study for SIDS endpoint

18.10.2006

### 5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

**Method** :
**Year** : 2003
**GLP** :
**Test substance** : other TS: Dissociation products

**Remark** : Aluminum distearate is expected to readily dissociate to Aluminum and Stearic acid.
Developmental effects data were not located for Stearic Acid.
Species: rat
Sex: female
Strain: other: Holtzmann
Route of admin.: i.p.
Exposure period: days 9-13 or 14-18 of gestation
Frequency of treatm.: 5 times
Duration of test: 20 days
Doses: 0; 75; 100; 200 mg/kg (AlCl3 crystals solved in sterile dist.water)
Control group: yes, concurrent no treatment
Remark: Maternal tox.:
- Dose dependent death in 100- and 200 mg/kg group;
- Stat. sign. differences in maternal weight gain at dose level 75 and 100 (treated on days 14-18 of gestation).
- In many cases maternal liver was severely damaged (perihepatic granulomas, signs of centrilobular necrosis).
Result: Offsprings treated with AlCl3 showed sign growth retardation as well as skeletal defects; incidence of fetal death and resorption was significantly increased.
75 mg/kg (day 14-18 of gestation): no malformation
There was no clear dose-response relationship respect to mean weight and length of fetuses.
100 mg/kg (day 14-18 of gestation): Three fetuses (from 2 litters) had abnormal digits.
7 fetuses (from 4 litters) had wavy ribs - in cases ribs were missing.
A large number of fetuses showed poor ossification (cranid bones, lower part of vertebral column, bones of limbs).
200 mg/kg: High incidence of dead offspring
Test Substance: aluminum chloride
Source: BASF AG Ludwigshafen as cited in ECB IUCLID (2000)
Reliability: (4) not assignable
Reference: Benett R.W. et al.: Anat.Anz. 138, 365-378, (1975) as cited in ECB IUCLID (2000)igElinder C.-G. and Sjoegren B. in: Friberg L.(Ed.) et al.: Handbook on the Toxicology Metals, 2nd. Ed., 1-25, Elsevier, (1986) as cited in ECB IUCLID (2000)

**Reliability** : (2) valid with restrictions
**Flag** : Critical study for SIDS endpoint
18.10.2006

### 5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

### 5.9 SPECIFIC INVESTIGATIONS

### 5.10 EXPOSURE EXPERIENCE

### 5.11 ADDITIONAL REMARKS

## 6.1 ANALYTICAL METHODS

## 6.2 DETECTION AND IDENTIFICATION

## 7.1 FUNCTION

## 7.2 EFFECTS ON ORGANISMS TO BE CONTROLLED

## 7.3 ORGANISMS TO BE PROTECTED

## 7.4 USER

## 7.5 RESISTANCE

## 8.1 METHODS HANDLING AND STORING

## 8.2 FIRE GUIDANCE

## 8.3 EMERGENCY MEASURES

## 8.4 POSSIB. OF RENDERING SUBST. HARMLESS

## 8.5 WASTE MANAGEMENT

## 8.6 SIDE-EFFECTS DETECTION

## 8.7 SUBSTANCE REGISTERED AS DANGEROUS FOR GROUND WATER

## 8.8 REACTIVITY TOWARDS CONTAINER MATERIAL

(1) EPIWIN v 3.11

(2) http://bulkpharm.mallinckrodt.com/_attachments/msds/ALUSD.htm

(3) Safepharm Laboratories (2006) ALUMINIUM STEARATE SEVEN DAY REPEATED DOSE ORAL (GAVAGE) TOXICITY STUDY IN THE RAT; SPL PROJECT NUMBER: 1683-0012

(4) SafePharm Laboratories (2007) Aluminium Stearates: Daphnia magna Reproduction Test. SPL Project Number 1683/0017

(5) Sax, N.I. and R.J. Lewis, Sr. (eds.). Hawley's Condensed

Chemical Dictionary. 11th ed. New York: Van Nostrand Reinhold Co., 1987.
46

## 10.1 END POINT SUMMARY

## 10.2 HAZARD SUMMARY

## 10.3 RISK ASSESSMENT

# IUCLID

# Data Set

| | | |
|---|---|---|
| **Existing Chemical** | : | ID: 637-12-7 |
| **CAS No.** | : | 637-12-7 |
| **EINECS Name** | : | aluminium tristearate |
| **EC No.** | : | 211-279-5 |
| **Molecular Formula** | : | C18H36O2.1/3Al |
| | | |
| **Producer related part** | | |
| **Company** | : | Epona Associates, LLC |
| **Creation date** | : | 06.12.2003 |
| | | |
| **Substance related part** | | |
| **Company** | : | Epona Associates, LLC |
| **Creation date** | : | 06.12.2003 |
| | | |
| **Status** | : | |
| **Memo** | : | SOCMA MCC |
| | | |
| **Printing date** | : | 07.12.2003 |
| **Revision date** | : | |
| **Date of last update** | : | 07.12.2003 |
| | | |
| **Number of pages** | : | 15 |
| | | |
| **Chapter (profile)** | : | Chapter: 2.1, 2.2, 2.4, 2.5, 2.6.1, 3.1.1, 3.1.2, 3.3.1, 3.5, 4.1, 4.2, 4.3, 5.1.1, 5.1.2, 5.1.3, 5.1.4, 5.4, 5.5, 5.6, 5.8.1, 5.8.2 |
| **Reliability (profile)** | : | Reliability: without reliability, 1, 2, 3, 4 |
| **Flags (profile)** | : | Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS |

## 2.1 MELTING POINT

| | | |
|---|---|---|
| **Value** | : | = 100 - 120 °C |
| **Sublimation** | : | |
| **Method** | : | |
| **Year** | : | 2002 |
| **GLP** | : | no data |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Test substance** | : | Purity = 100% |
| **Reliability** | : | (2) valid with restrictions |

06.12.2003 (3)

| | | |
|---|---|---|
| **Value** | : | = 117 - 120 °C |
| **Sublimation** | : | |
| **Method** | : | |
| **Year** | : | 2003 |
| **GLP** | : | no data |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Source** | : | Epona Associates, LLC |
| **Reliability** | : | (2) valid with restrictions<br>Information taken from a peer-reviewed source. |
| **Flag** | : | Critical study for SIDS endpoint |

06.12.2003 (7)

## 2.2 BOILING POINT

| | | |
|---|---|---|
| **Decomposition** | : | yes |
| **Method** | : | |
| **Year** | : | 2003 |
| **GLP** | : | |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Source** | : | Epona Associates, LLC |
| **Test substance** | : | Purity = 100% |
| **Reliability** | : | (2) valid with restrictions |
| **Flag** | : | Critical study for SIDS endpoint |

06.12.2003 (3)

## 2.4 VAPOUR PRESSURE

| | | |
|---|---|---|
| **Decomposition** | : | |
| **Method** | : | other (calculated) |
| **Year** | : | 2002 |
| **GLP** | : | no |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Result** | : | 1.08E-018 mm Hg (Modified Grain method) |
| **Source** | : | Epona Associates, LLC |
| **Reliability** | : | (3) invalid |
| **Flag** | : | Critical study for SIDS endpoint |

06.12.2003 (4)

## 2.5 PARTITION COEFFICIENT

| | | |
|---|---|---|
| **Partition coefficient** | : | octanol-water |
| **Log pow** | : | = 22.69 at °C |
| **pH value** | : | |
| **Method** | : | other (calculated) |
| **Year** | : | 2003 |
| **GLP** | : | no |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Remark** | : | Aluminum tristearate is expected to dissociate to aluminum and stearic acid. |
| **Source** | : | Epona Associates, LLC |
| **Reliability** | : | (3) invalid<br>Endpoint not applicable as the material is not soluble in water. |
| **Flag** | : | Critical study for SIDS endpoint |

06.12.2003 (2)

## 2.6.1 SOLUBILITY IN DIFFERENT MEDIA

| | | |
|---|---|---|
| **Solubility in** | : | Water |
| **Value** | : | at °C |
| **pH value** | : | |
| **concentration** | : | at °C |
| **Temperature effects** | : | |
| **Examine different pol.** | : | |
| **pKa** | : | at 25 °C |
| **Description** | : | not soluble |
| **Stable** | : | |
| **Deg. product** | : | |
| **Method** | : | |
| **Year** | : | 1983 |
| **GLP** | : | no data |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Source** | : | Epona Associates, LLC |
| **Reliability** | : | (2) valid with restrictions<br>Information taken from a peer-reviewed source. |

06.12.2003 (6)

| | | |
|---|---|---|
| **Solubility in** | : | Water |
| **Value** | : | at °C |
| **pH value** | : | |
| **concentration** | : | at °C |
| **Temperature effects** | : | |
| **Examine different pol.** | : | |
| **pKa** | : | at 25 °C |
| **Description** | : | |
| **Stable** | : | |
| **Deg. product** | : | |
| **Method** | : | other: calculated |
| **Year** | : | 2003 |
| **GLP** | : | no |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Result** | : | Water Solubility Estimate from Log Kow (WSKOW v1.41):<br>Water Solubility at 25 deg C (mg/L): 9.386e-020 |
| **Source** | : | Epona Associates, LLC |
| **Reliability** | : | (3) invalid |

Endpoint not applicable as the material is not soluble in water.

06.12.2003 (2)

### 3.1.1 PHOTODEGRADATION

| | | |
|---|---|---|
| **Type** | : | air |
| **Light source** | : | |
| **Light spectrum** | : | nm |
| **Relative intensity** | : | based on intensity of sunlight |
| **DIRECT PHOTOLYSIS** | | |
| **Halflife t1/2** | : | = .2 day(s) |
| **Degradation** | : | % after |
| **Quantum yield** | : | |
| **INDIRECT PHOTOLYSIS** | | |
| **Sensitizer** | : | |
| **Conc. of sensitizer** | : | |
| **Rate constant** | : | = .000000000064 cm³/(molecule*sec) |
| **Degradation** | : | - % after |
| **Deg. product** | : | |
| **Method** | : | other (calculated) |
| **Year** | : | 2003 |
| **GLP** | : | no |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |

**Result** : Atmospheric Oxidation (25 deg C) [AopWin v1.91]:
Hydroxyl Radicals Reaction:
OVERALL OH Rate Constant = 64.3647 E-12 cm3/molecule-sec
Half-Life = 0.166 Days (12-hr day; 1.5E6 OH/cm3)
Half-Life = 1.994 Hrs
Ozone Reaction:
No Ozone Reaction Estimation

| | | |
|---|---|---|
| **Source** | : | Epona Associates, LLC |
| **Reliability** | : | (2) valid with restrictions |
| **Flag** | : | Critical study for SIDS endpoint |

06.12.2003 (2)

### 3.1.2 STABILITY IN WATER

| | | |
|---|---|---|
| **Deg. product** | : | |
| **Method** | : | |
| **Year** | : | 2003 |
| **GLP** | : | no |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |

**Remark** : Aluminum tristearate is not soluble in water.
The hydrolysis data for the dissociation products is: "unstable" (aluminum chloride) and not avaiable due to low water solubility (stearic acid)

| | | |
|---|---|---|
| **Source** | : | Epona Associates, LLC |
| **Reliability** | : | (2) valid with restrictions |
| **Flag** | : | Critical study for SIDS endpoint |

07.12.2003

### 3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

| | | |
|---|---|---|
| **Type** | : | fugacity model level III |
| **Media** | : | |
| **Air** | : | % (Fugacity Model Level I) |
| **Water** | : | % (Fugacity Model Level I) |
| **Soil** | : | % (Fugacity Model Level I) |

**Biota** : % (Fugacity Model Level II/III)
**Soil** : % (Fugacity Model Level II/III)
**Method** : other: estimated
**Year** : 2003

**Result** : Level III Fugacity Model:

| | Mass Amount (percent) | Half-Life (hr) | Emissions (kg/hr) |
|---|---|---|---|
| Air | 0.0598 | 3.99 | 1000 |
| Water | 2.35 | 1.44e+003 | 1000 |
| Soil | 29.9 | 1.44e+003 | 1000 |
| Sediment | 67.7 | 5.76e+003 | 0 |

Persistence Time: 2.61e+003 hr

**Source** : Epona Associates, LLC
**Reliability** : (2) valid with restrictions
**Flag** : Critical study for SIDS endpoint
06.12.2003 (2)

## 3.5 BIODEGRADATION

**Deg. product** :
**Method** : other: calculated
**Year** : 2003
**GLP** : no
**Test substance** : as prescribed by 1.1 - 1.4

**Remark** : Aluminum tristearate is not soluble in water.
The biodegradation of the dissociation products are: not applicable - unstable in water (aluminum chloride) and readily biodegradable (Stearic acid).

**Result** : Probability of Rapid Biodegradation (BIOWIN v4.01):
Linear Model : 0.6551
Non-Linear Model : 0.0195
Expert Survey Biodegradation Results:
Ultimate Survey Model: 2.1552 (months )
Primary Survey Model : 3.3890 (days-weeks )
Readily Biodegradable Probability (MITI Model):
Linear Model : 0.4750
Non-Linear Model : 0.1062

**Source** : Epona Associates, LLC
**Reliability** : (3) invalid
Endpoint not applicable as the material is not soluble in water.
07.12.2003 (2)

## 4.1 ACUTE/PROLONGED TOXICITY TO FISH

**Method** :
**Year** : 2003
**GLP** :
**Test substance** : other TS: Dissociation products

**Remark** : Aluminum tristearate is not soluble in water, and is expected to readily dissociate to Aluminum and Stearic acid.
Species:Oncorhynchus mykiss (Fish, fresh water)
Exposure period 96 hour(s)
Unit: mg/l
LC50: = 8.6
Test Substance: Aluminum chloride
Reference: Call, DJ, LT Brooke, CA Lindberg, TP MArkee, DJ MaCauley, and SH Poirier (1984) Toxicity of Aluminum to Freshwater Organisms in Water of pH 6.5-8.5. Tech Rep Project No. 549-238-RT-WRD, Center for Lake Superior Environmental Studies, University of Wisconsin, Superior, WI. /November 27, 1984 Memo to C Stephan, USEPA, Duluth, MN:46 p (Author Communication Used).

Type:static
Species:Oncorhynchus kisutch (Fish, fresh water, marine)
Exposure period:96 hour(s)
Unit: µg/l
LC50: = 12000 - measured/nominal
Method:
Year: 1977
GLP: no data
Test substance: Stearic acid

Test substance: "pure"
Reliability: (2) valid with restrictions
Flag: Critical study for SIDS endpoint
Reference: SIDS Leach, J.M. and A.N. Thakore (1977)
Compounds Toxic to Fish Pulp Mill Waste Streams Progress in Water Technology, 9: 787-798 CIS Record ID.: AQ-0132049

**Source** : Epona Associates, LLC
**Reliability** : (2) valid with restrictions
07.12.2003

## 4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

**Method** :
**Year** : 2003
**GLP** :
**Test substance** : other TS: Dissociation products

**Remark** : Acute toxicity to aquatic invertebrates was not located for stearic acid. Aluminum tristearate is not soluble in water, and is expected to readily dissociate to Aluminum and Stearic acid.
Type:static
Species other: Ceriodaphnia dubia
Exposure period : 48 hour(s)
Unit: mg/l
EC50: = 1.5 - measured/nominal
Method:

Year: 1986
GLP: no data
Test substance: as prescribed by 1.1 - 1.4

Test condition: Water Parameters:
Temperature (TMP): 25.3 (mean value); Units: C
Dissolved O2 (mg/l or % saturation) (DO2): 7.3 (mean value) mg/L
pH: 7.86 (mean value)

Test substance: Aluminum chloride, 99.8% purity
Reliability: (2) valid with restrictions
Information taken from a peer-reviewed publication.
Flag: Critical study for SIDS endpoint
Reference: McCauley, D.J., L.T. BROOKE, D.J. CALL and C.A. LINDBERG (1986) Acute and Chronic Toxicity of Aluminum to Ceriodaphnia dubia at Various pH's. Center for Lake Superior Environmental Studies, University of Wisconsin, Superior, WI: 15; 1986
CIS Record ID.: AQ-0113175

**Source** : Epona Associates, LLC
**Reliability** : (2) valid with restrictions
07.12.2003

### 4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

**Method** :
**Year** : 2003
**GLP** :
**Test substance** : other TS: Dissociation products

**Remark** : Acute toxicity to aquatic invertebrates or aquatic plants was not located for stearic acid or aluminum chloride.
Aluminum distearate is not soluble in water, and is expected to readily dissociate to Aluminum and Stearic acid.

**Reliability** : (2) valid with restrictions
07.12.2003

### 5.1.1 ACUTE ORAL TOXICITY

**Method** :
**Year** : 2003
**GLP** :
**Test substance** : other TS: Dissociation products

**Remark** : Aluminum tristearate is expected to readily dissociate to Aluminum and Stearic acid.
Type: LD50
Value: = 370 - mg/kg bw
Species: rat
Strain: Sprague-Dawley
Year: 1987
GLP: no data
Test substance: Aluminum chloride
Reliability: (2) valid with restrictions
Information taken from a peer-reviewed publication.
Flag: Critical study for SIDS endpoint
Reference: Agency for Toxic Substances and Disease Registry [ATSDR] 1999, Toxicological Profile for Alumunim; and Llobet JM, Domingo JL, Gomez M, et al. 1987. Acute toxicity studies of aluminum compounds: Antidotal efficacy of several chelating agents. Pharmacol Toxicol 60:280-283.Liobet et al (1987)

Type: LD50
Value: = 4600 - mg/kg bw
Species: rat
GLP: no data
Test substance: stearic acid
Reliability: (2) valid with restrictions
Information taken from a peer-reviewed publication.
Reference: Clayton, G.D., F.E. Clayton (eds.) Patty's Industrial Hygiene and Toxicology. Volumes 2A, 2B, 2C, 2D, 2E, 2F: Toxicology. 4th ed. New York, NY: John Wiley & Sons Inc., 1993-1994. 3568. Cited in BiblioLine

**Source** : Epona Associates, LLC
**Reliability** : (2) valid with restrictions
**Flag** : Critical study for SIDS endpoint
07.12.2003

### 5.1.2 ACUTE INHALATION TOXICITY

### 5.1.3 ACUTE DERMAL TOXICITY

### 5.1.4 ACUTE TOXICITY, OTHER ROUTES

### 5.4 REPEATED DOSE TOXICITY

**Method** :
**Year** : 2003
**GLP** :
**Test substance** : other TS: Dissociation products

**Remark** : Aluminum tristearate is expected to readily dissociate to Aluminum and Stearic acid.
Type: Sub-acute
Species: mouse
Sex: female
Strain: Swiss Webster
Route of admin.: oral feed
Exposure period: other: 5 or 7 weeks
NOAEL: = 195 - mg/kg bw
Year: 1993
GLP: no data
Test substance: Aluminum chloride

Remark: Approximate feed concentrations of 250 and 350 ppm aluminum (ATSDR, 1999)
Result: Mice that ingested doses higher than 130 mg Al/kg/day as aluminum chloride for 49 days, and were tested
using a standardized neurotoxicity screening battery, also showed decreased motor activity, as well as
decreased grip strength and startle responsiveness.
Signs of neurotoxicity but no change in hematocrit levels, no liver changes at 195 mg/kg/day. No body weight chnages at 260 mg/kg/day.
Test condition: Adult mice consumed aluminum chloride for 5-7 weeks in a diet that also contained 3.5% sodium citrate.
Reliability: (2) valid with restrictions
Information taken from a peer-reviewed publication.
Reference: Agency for Toxic Substances and Disease Registry [ATSDR] 1999, Toxicological Profile for Aluminum; and Oteiza PI, Keen CL, Han B, et al. 1993. Aluminum accumulation and neurotoxicity in Swiss-mice after long-term dietary exposure to aluminum and citrate. Metabolism 42:1296-1300.

Type: Sub-chronic
Species: rat
Route of admin.: oral feed
Exposure period: 24 weeks
Doses: 50g/kg/day
GLP: no data
Test substance: Stearic acid

Result: Rats fed 50 g/kg/day stearic acid for 24 weeks developed reversible lipogranulomas in adipose tissue. No significant pathological lesions were observed in rats fed 3000 ppm stearic acid orally for about 30 weeks, but anorexia, increased mortality, and a greater incidence of pulmonary infection were observed. Stearic acid is one of the least effective fatty acids in producing hyperlipemia, but the most potent in diminishing blood clotting time.
Reliability: (2) valid with restrictions
Information taken from a peer-reviewed publication.
Reference: Clayton, G.D., F.E. Clayton (eds.) Patty's Industrial Hygiene and Toxicology. Volumes 2A, 2B, 2C, 2D, 2E, 2F: Toxicology. 4th ed. New York, NY: John Wiley & Sons Inc., 1993-1994. 3568. Cited in BiblioLine

**Source** : Epona Associates, LLC
**Reliability** : (2) valid with restrictions
**Flag** : Critical study for SIDS endpoint
07.12.2003

## 5.5 GENETIC TOXICITY ‘IN VITRO‘

| | | |
|---|---|---|
| **Type** | : | |
| **System of testing** | : | |
| **Test concentration** | : | |
| **Cycotoxic concentr.** | : | |
| **Metabolic activation** | : | |
| **Result** | : | |
| **Method** | : | |
| **Year** | : | 2003 |
| **GLP** | : | |
| **Test substance** | : | other TS: Dissociatin products |

**Remark** :

Aluminum tristearate is expected to readily dissociate to Aluminum and Stearic acid.
Genotoxicity data were not located for Stearic Acid.
Multiple studies with bacterial systems indicate aluminum chloride is not a bacterial mutagen. This is one of several studies sumamrized in the Aluminum chloride IUCLID.
Type: Ames test
System of testing: Salmonella typhimurium TA1537 TA2637 TA98 TA100 TA102
Test concentration:
Result: negative
Year: 1987
GLP: no data
Test substance: Aluminum chloride
Source: BASF AG Ludwigshafen as cited in ECB IUCLID (2000)
Reliability: (4) not assignable
Reference: Ogawa H.I. et al.: Jpn.J.Genet. 62, 159-162, (1987)

Multiple studies with in vitro mammalian systems indicate aluminum chloride is not genotoxic. This is one of several studies sumamrized in the Aluminum chloride IUCLID.

Type: Mouse lymphoma assay
System of testing: L5178Y TK+/- Mouse Lymphoma cells
Test concentration: 570, 580, 590, 600, 620, 625 ug/ml
Metabolic activation: with and without
Result: negative
Method: other: according to Clive, D. et al.: Mutat. Res. 59, 61-108
Year: 1979
GLP: no data
Test substance: Aluminum chloride
Remark: forward mutation assay with and without metabolic activationwith S9-mix prepared from liver homogenate of Aroclor pretreated Sprague-Dawley rats; the mutation frequency remained constant at ca. 2-fold
Source: BASF AG Ludwigshafen as cited in ECB IUCLID (2000)
Test substance: aluminium chloride; according to the authors, the compound was of certified ACS grade
Reliability: (4) not assignable
Original study not reviewed.
Reference: Oberly T.J. and Piper C.E.: Environ. Mutag. 2, 281 (1980); abstract as cited in ECB IUCLID (2000); and Oberly T.J. et al.: J. Toxicol. Environ. Health 9, 367-376 (1982) as cited in ECB IUCLID (2000)

| | | |
|---|---|---|
| **Reliability** | : | (2) valid with restrictions |
| **Flag** | : | Critical study for SIDS endpoint |

07.12.2003

## 5.6 GENETIC TOXICITY ‘IN VIVO‘

| | | |
|---|---|---|
| **Type** | : | |
| **Species** | : | |
| **Sex** | : | |
| **Strain** | : | |
| **Route of admin.** | : | |
| **Exposure period** | : | |
| **Doses** | : | |
| **Result** | : | |
| **Method** | : | |
| **Year** | : | 2003 |
| **GLP** | : | |
| **Test substance** | : | other TS: Dissociation products |

**Remark** :

Aluminum tristearate is expected to readily dissociate to Aluminum and Stearic acid.
Genotoxicity data were not located for Stearic Acid.
Type: Micronucleus assay
Species: mouse
Route of admin.: i.p.
Exposure period : bone marrow cells were fixed at times up to 72 h
Doses: .01, .05 or .1 molar aluminum chloride
Result: positive
Year: 1972
GLP: no data
Test substance: Aluminum chloride
Result: "There was a significant
increase in chromatid-type aberrations over the controls, and these occurred in a nonrandom distribution
over the chromosome complement. No dose-response relationship could be demonstrated, although the highest dose of aluminum chloride did produce the greatest number of aberrations." (ATSDR, 1999)
The effect was qualitatively more or less the same at
different intervals as well as at different concentrations
in the form of erosion, stickiness, etc. as general and
subchromatid, chromatid and chromosome breaks,
ranslocations, gaps and constrictions in the individual
chromosomes.
Source: BASF AG Ludwigshafen as cited in ECB IUCLID (2000) Epona Asociates, LLC
Test condition: Mice were injected intraperitoneally with 0.01, 0.05, or 0.1 molar aluminum
chloride, and bone marrow cells were examined for chromosomal aberrations.
Reliability: (2) valid with restrictions
Flag: Critical study for SIDS endpoints.
Reference: Agency for Toxic Substances and Disease Registry [ATSDR] 1999, Toxicological Profile for Aluminum; and Manna GK, Das RK. 1972. Chromosome aberrations in mice induced by aluminum chloride. Nucleus 15:180-186.

| | | |
|---|---|---|
| **Source** | : | Epona Associates, LLC |
| **Reliability** | : | (2) valid with restrictions |
| **Flag** | : | Critical study for SIDS endpoint |

07.12.2003

### 5.8.1 TOXICITY TO FERTILITY

| | | |
|---|---|---|
| **Method** | : | |
| **Year** | : | 2003 |
| **GLP** | : | |

**Test substance** : other TS: Dissociation products

**Remark** : Aluminum tristearate is expected to readily dissociate to Aluminum and Stearic acid.
Effects on fertilitydata were not located for Stearic Acid.
Type: other: three generation
Species: mouse
Strain: Swiss Webster
Route of admin.: other: drinking water and base diet
Exposure period: 180 - 390 d (weanlings were treated from 4.week of age like parents)390 days
No. of generation studies: 3
Doses: 0; 19.3 mg/kg/d (doses expressed in terms of Al)
Result: no effects on fertility
Year: 1966
GLP: no data
Test substance: Aluminum chloride
Remark: "Aluminum apparently does not affect reproduction. Finally, pharmacokinetic data do not indicate that the reproductive organs are target organs" (ATSDR, 1999)
Result: There were no significant differences in the numbers of litters or off-spring between the treated and control mice. Growth was retarded and was dependent on the intake of aluminium, but the effect did not appear in the first generation or in the first litter. The subsequent litters manifested a very marked growth retardation, as did those of the third generation. An analysis of variance established that, under the conditions of our experiment, weight variations could be accounted for by aluminium uptake ($P < 0.001$). The differences in the course of weight plots for successive generations and litters were also statistically significant ($P < 0.01$).
The erythrocyte counts and haemoglobin levels in the first and last generations did not differ significantly from those in the controls; and no pathological changes could be found in the tissues examined.
Source: BASF AG Ludwigshafen as cited in ECB IUCLID (2000)
Reliability: (2) valid with restrictions
Reference: Agency for Toxic Substances and Disease Registry [ATSDR] 1999, Toxicological Profile for Aluminum; and Ondreicka R, Ginter E, Kortus J. 1966. Chronic toxicity of aluminum in rats and mice and its effects on phosphorus metabolism Br J Ind Med 23:305-312.

**Source** : Epona Associates, LLC
**Reliability** : (2) valid with restrictions
**Flag** : Critical study for SIDS endpoint
07.12.2003

### 5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

**Method** :
**Year** : 2003
**GLP** :
**Test substance** : other TS: Dissociation products

**Remark** : Aluminum tristearate is expected to readily dissociate to Aluminum and Stearic acid.
Developmental effects data were not located for Stearic Acid.
Species: rat
Sex: female
Strain: other: Holtzmann

Route of admin.: i.p.
Exposure period: days 9-13 or 14-18 of gestation
Frequency of treatm.: 5 times
Duration of test: 20 days
Doses: 0; 75; 100; 200 mg/kg (AlCl3 crystals solved in sterile dist.water)
Control group: yes, concurrent no treatment
Remark: Maternal tox.:
- Dose dependent death in 100- and 200 mg/kg group;
- Stat. sign. differences in maternal weight gain at dose level 75 and 100 (treated on days 14-18 of gestation).
- In many cases maternal liver was severely damaged (perihepatic granulomas, signs of centrilobular necrosis).
Result: Offsprings treated with AlCl3 showed sign growth retardation as well as skeletal defects; incidence of fetal death and resorption was significantly increased.
75 mg/kg (day 14-18 of gestation): no malformation
There was no clear dose-response relationship respect to mean weight and length of fetuses.
100 mg/kg (day 14-18 of gestation): Three fetuses (from 2 litters) had abnormal digits.
7 fetuses (from 4 litters) had wavy ribs - in cases ribs were missing.
A large number of fetuses showed poor ossification (cranid bones, lower part of vertebral column, bones of limbs).
200 mg/kg: High incidence of dead offspring
Test Substance: aluminum chloride
Source: BASF AG Ludwigshafen as cited in ECB IUCLID (2000)
Reliability: (4) not assignable
Reference: Benett R.W. et al.: Anat.Anz. 138, 365-378, (1975) as cited in ECB IUCLID (2000)igElinder C.-G. and Sjoegren B. in: Friberg L.(Ed.) et al.: Handbook on the Toxicology Metals, 2nd. Ed., 1-25, Elsevier, (1986) as cited in ECB IUCLID (2000)

**Source** : Epona Associates, LLC
**Reliability** : (2) valid with restrictions
**Flag** : Critical study for SIDS endpoint
07.12.2003

(2) EPIWIN v. 3.11

(3) Mallinckrodt Inc. (2002) Material Data Safety Sheet Aluminum Tristearate 3/13/2002

(4) MPBPWIN v1.41

(6) The Merck Index. 10th ed. Rahway, New Jersey: Merck Co., Inc., 1983. 54

(7) The Merck Index. 10th ed. Rahway, New Jersey: Merck Co., Inc., 1983. 54

# U.S. High Production Volume (HPV) Chemical Challenge Program

201-16572E

# FINAL SUBMISSION: ALUMINUM STEARATES CATEGORY

**The Metal Carboxylates Coalition**

**A SOCMA Affiliated Consortium**

**JANUARY 2007**

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## SUMMARY

The Metal Carboxylates Coalition has sponsored 20 compounds that are metal salts of carboxylic acids under the HPV Challenge Program. Metal Carboxylates are metal salts of carboxylic acids. These compounds readily dissociate to the corresponding metal and carboxylic acid. The HPV endpoints are fulfilled using a combination of data from the parent molecule, as well as for the dissociation products; that is, a metal salt and/or a carboxylic acid. Selected testing of the parent molecules was proposed and completed to further fulfill HPV endpoints. Robust summaries are provided for the parent molecules as well as the dissociation products.

This final submittal provides the information relevant to the HPV Challenge Program for the aluminum distearates category:

| | |
|---|---|
| Aluminum Distearate | 300-92-5 |
| Aluminum Tristrearate | 637-12-7 |

# 1.0 BACKGROUND

This final submittal provides the information relevant to the HPV Challenge Program for the aluminum distearates category:

| | |
|---|---|
| Aluminum Distearate | 300-92-5 |
| Aluminum Tristrearate | 637-12-7 |

Figure 1 provides structures of these two related materials.

## 1.1 Use Patterns for Metal Carboxylates

The metal carboxylates function to deliver a metal ion into chemical reactions. The carboxylic acids (acids) are tailored for use in different products or chemical reactions.

## 1.2 Common Characteristics of Metal Carboxylates

These two metal carboxylates (aluminum di- and tri-stearate) are functionally similar and have the same ionizable substituents, the same metal cation, and a structurally similar carboxylic acid group (RCOOH). These compounds are divalent compounds and have two carboxylic acid moieties per molecule. The metal carboxylate salts are designed to add metals to chemical reactions; therefore, they are designed to readily dissociate into the free metal and free acid.

# 2.0 Dissociation Studies

One key characteristic of metal carboxylates is that they readily dissociate from an ion pair into free metal and free acid. They are found as partially dissociated products in the ambient environment (i.e., neutral pH). Dissociation is a reversible process and the portion of dissociated salt present is dependent on the pH and pKa (the dissociation constant), which is the pH at which 50% dissociation occurs. In the low pH environment of the digestive tract (e.g., pH 1.2) complete dissociation will occur for these metal carboxylates. The transport and bioavailability of the metals and acids are determined by their solubility in environmental media and biological fluids which is determined by environmental parameters such as pH.

Completion of the dissociation study with these two aluminum stearate compounds was not possible due to low water solubility, although these compounds are expected to readily dissociate (Crompton Corporation, personal communication). Studies with other metal carboxylates indicate that significant dissociation will occur at approximately neutral pH (i.e., representative of aquatic and marine ecosystems), while complete dissociation will occur at physiologically relevant pH of the mammalian stomach (pH 1.2). These findings are particularly important in relating available data for the respective acids and metals to support

the existing data for aluminum di- and tri-stearate and in the fulfillment of critical endpoints.

Dissociation is a reversible reaction, splitting the parent compound into two or more chemical species which may be ionic, but are not necessarily so. The process can be generally represented as:

High pH Low pH

$$[RCOO^-]_x:[M^+]_x \leftrightarrow [RCOO^-]_x + [M^+]_x \leftrightarrow [RCOOH]_x + [MCl]_x$$

(salt) (Titrate with HCl →) free acid and free metal

The pKa and pH are equal when the metal carboxylate salt is 50% dissociated. The parent compounds, the metal carboxylate salts, are associated ionized molecules.

The dissociation constant is important for two reasons. First, it determines the proportion of any specific acid or metal that is dissociated at a given pH. The free acid and corresponding free metal are often much different than the salt (ion pair) moiety in characteristics such as solubility, adsorption, and toxicity. The proportion of dissociation influences the behavior of the substance in the environment and bioavailability of the acid and metal constituents of metal carboxylate salts.

The dissociation constants for 18 related metal carboxylate compounds tested have pKa (pKb) values (pKa1) in the neutral range (5.088 to 8.448). This indicates that in the neutral pH range, significant portions of the metal carboxylates will be dissociated. In addition, at the low pH of the mammalian stomach (pH 1.2) all of the metal carboxylates would be expected to be completely or nearly completely dissociated. This indicates that the absorption and any observed toxicity would be independent for the respective acid and metal when administered orally.

The dissociation constants show that at the pH of the stomach and at the pH of environmental media the important moieties are the ionized free acid and metal. Because of this, environmental fate, ecotoxicity, and mammalian toxicity of the free acid, or that for a simple salt (e.g., the sodium salt), can to serve as a surrogate data for the acid component of respective metal carboxylates. Similarly, under these conditions, data for the metal ion can be represented by fate and toxicity data on of free metal ion or simple metal salts (e.g., metal chlorides). Therefore, the role in any observed toxicity for acids and metals can be evaluated independently (i.e., as the free metal and/or free acid).

To the extent they are soluble, aluminum stearates dissociate; however, attempts to quantity dissociation, i.e., to develop a Dissociation Constant, were unsuccessful because of limited water solubility. As pointed out by EPA, the Ko/w

of aluminum tristearate is 22.7, suggesting that it is a very lipid soluble compound. A portion of the bioavailability of this Aluminum Stearate is driven by dissociation products and an apparently larger portion is driven by undissociated carboxylate. The ratio of dissociated species to undissociated Aluminum stearate species is less clear than with other metal carboxylates; what is clear is the low systemic toxicity issuing from each of the Aluminum Stearates species. Results of the 7-day repeated dosing studies in rats (described in Section 5.0) confirm that systemic toxicity of Aluminum Stearates is low.

## 3.0 Bioequivalency

The work described below by Stopford et al. (unpublished)[1] shows that the metal chloride is similar to, or more bioavailable than, the corresponding metal carboxylate salts, which makes the chloride a conservative surrogate in estimating bioavailability and toxicity of dissociated metals. Chlorides of the various metals have been emphasized during preparation of the attached robust summaries and are the preferred surrogate data for carboxylate salts.

Recent studies conducted to evaluate the "bioequivalency" (an estimate of bioavailability) of cobalt compounds, included three cobalt carboxylates and cobalt chloride. The solubility of these compounds in synthetic biological fluids (gastric juices, intestinal juices, several interstitial fluids, and cytosol) showed that these salts were completely dissociated and dissolved at gastric pH and cytosolic pH. The dissolution of these compounds ranged from 26.1% to 80.4 % of available cobalt at neutral pH (Table 1). The results for cobalt chloride and cobalt 2-ethyl-hexanoate were very similar at acidic and neutral pH. Cobalt neodecanoate and cobalt naphthenate showed similar levels of dissolution at acidic (gastric and cytosolic) pH, but smaller proportions of the metal component of these compounds were dissolved at neutral pH. The differences in dissolution for these metal carboxylates at neutral pH in synthetic body fluids could be related to differences in their dissociation constants.

These data are valuable in understanding the aluminum stearates for three reasons:

1. They confirm the prediction that these stearate compounds would be expected to be completely dissociated in the gastrointestinal tract (low pH) and a substantial proportion of these compounds would be expected to be dissociated and bioavailable at neutral pH (7.4).

[1] Stopford, W., J. Turner, D. Cappellini, and T. Brock. (unpublished) Bioequivalency Testing of Cobalt Compounds (Oct 15, 2002 Draft). Conducted by Duke University Medical Center, Division of Occupational and Environmental Medicine for the Cobalt Development Institute, Research Triangle Park, N.C.

2. The fraction of the three cobalt carboxylates that is dissolved at acidic and neutral pH is very similar for different acid constituents with a range of molecular weights and chain lengths. This finding greatly strengthens the extrapolation of the results to the aluminum stearates.

3. The work by Stopford et al. (unpublished) shows that the metal chloride is similar to, or more bioavailable than, the corresponding metal carboxylate salts, which makes the chloride a conservative surrogate in estimating bioavailability and toxicity of dissociated metals. Chlorides of the various metals have been emphasized during preparation of the attached robust summaries and are the preferred surrogate data for carboxylate salts.

## 4.0 Supporting Data for Aluminum Stearates and their Dissociation Products

Data for the aluminum stearates (Appendix C and D) and their dissociation products (aluminum chloride and Stearic acid, Appendix A and B, respectively) are provided in robust summary format.

Consistent with discussions between the Metal Carboxylates Coalition and the EPA, data for the dissociation products (metals and acids) are recognized as being essential to understanding the environmental fate and toxicological characteristics of the respective metal carboxylate salts. Data for stearic acid and aluminum are useful in characterizing the hazard of the aluminum stearate compounds.

In summary, the key points relative to the two aluminum stearates are:

- Dissociation to stearic acid and aluminum (described as aluminum chloride);
- Expected Dissociation constants (pKa) in the circum neutral range (5.088 to 8.448);
    - Complete or nearly complete dissociation at gastric and cytosolic pH levels;
    - A moderate to high proportion of dissociation in the neutral pH range;
- General bioequivalency for salts with the same metal cation (cobalt used as an example within this document) and different acids or the chloride salt;
- Aluminum stearates have the same use pattern, to provide free metal ion to chemical reactions.
- Provision of data for the parent molecule or one or both of its dissociation products

## 5.0 Completed Test Plan

The aluminum stearates are the high molecular weight compounds (~610 for aluminum distearate and ~877 for aluminum tristearate). The Metal Carboxylates Coalition has relied on the fact that these compounds will dissociate and that the respective acid (stearic acid), and metal (aluminum) are the chemicals of interest. Although dissociation was not demonstrated as these materials have water solubilities too low to allow analysis by the standard methods (OECD Guideline 112), these two compounds are expected to dissociate readily in water at neutral pH's and to be completely dissociated at the pH of the stomach (pH 1.2) as demonstrated for other metal carboxylates.

Stearic acid has a long history of safe use in foods and cosmetics. This compound is sponsored by the Aliphatic Acids Category under the HPV Challenge Program.

The Metal Carboxylates Coalition is relying on the data for stearic acid and aluminum to support these two materials and to minimize unnecessary testing. The Coalition has prepared a robust summary document for stearic acid which describes the necessary endpoint data under the HPV Program (Appendix A). More complete or more robust data may become available following submission of the Aliphatic Acids Category to the EPA under the HPV Challenge Program by the Soap and Detergents Association. A robust summary document has also been prepared for aluminum chloride (Appendix B).

Physicochemical Properties:

Table 2 provides a summary of the physical chemical data for the aluminum stearates, as well as their dissociation products. Melting point data are available for both materials. Both are expected to decompose such that a boiling point test is not necessary. Vapor pressures are anticipated to be very low (modeling data indicate vapor pressures will be in the range of 4E-17 mm Hg (distearate) to 1.08E-18 mm Hg (tristearate). The water solubility of these materials is very low (nearly insoluble).

*The physical chemical properties endpoints are complete.*

Environmental Fate:

Table 2 provides a summary of the environmental fate data for the aluminum stearates, as well as their dissociation products. Most tests of environmental fate (partition coefficient, stability in water and biodegradation) are not appropriate for these materials due to their very low water solubility. Model estimates of these parameters are presented in Table 2. Partition coefficient and biodegradation studies are available for stearic acid, which is considered to be representative of the two materials since these compounds dissociate and stearic acid will be the

moiety of interest. Stearic acid is readily biodegradable, and has a partition coefficient of >8. Photodegradation and transport (fugacity) have been calculated using SAR models (e.g., EPIWIN) for the aluminum stearates.

*The environmental fate endpoints are complete.*

Environmental Effects:

Table 2 provides a summary of the environmental effects data for the aluminum stearates, as well as their dissociation products. Due to the very low water solubility of these materials, as well as the low water solubility of stearic acid, acute aquatic toxicity tests are not expected to be relevant. A chronic daphnia test (OECD TG 211) with aluminum distearate was conducted. The 14- and 21-day EC50 (immobilization) values, based on nominal test concentrations for the parental Daphnia generation (P1) were calculated to be 0.24 and 0.048 mg/L; The 21-day EC50 (reproduction) value based on nominal test concentrations was calculated to be 0.059 mg/L. The LOEC was 0.020 mg/L and the NOEC was 0.0061 mg/L.

*The environmental effects endpoints are complete.*

Human Health Effects:

Data elements for human health effects endpoints were examined for the aluminum stearates, stearic acid and aluminum (Table 2). Mammalian toxicity is represented by data available for the dissociation products and by a 7 day gavage study in rats with aluminum distearate. Aluminum distearate was administered by gavage to five rats/sex/group to 0, 150, 500 and 1000 mg/kg/day for seven consecutive days. There was a transient reduction in bodyweight gain for females treated with 1000 mg/kg/day. In the absence clinical signs of toxicity, this transient effect on bodyweight gain was considered not to have a detrimental effect on the health of the animals. The NOAEL was 1000 mg/kg/day.

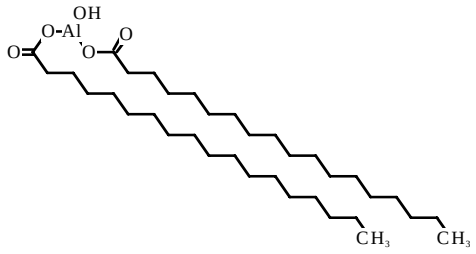
*The human health effects endpoints are complete.*

## 5.1 SUMMARY

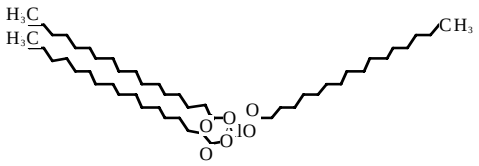
The Metal Carboxylates Coalition commitment to the USEPA HPV Challenge Program for the aluminum stearates category is complete.

# FIGURES

***Figure 1: Structures***




MolWt: 610.95 C36 H71 O5 Al1
000300-92-5 Aluminum, hydroxybis(octadecanoato-O)-




MolWt: 877.42 C54 H105 O6 Al1
000637-12-7 Aluminum stearate

# TABLES

**Table 1: Results of Extraction of Cobalt from Surrogate Biological Fluids**

| **Matrix (pH)** | **Maximum Solubility (% of available metal)** | | | |
|---|---|---|---|---|
| | $CoCl_2$ | Co 2-ethyl-hexanoate | Co naphthenate | Co neodecanoate |
| Gastric pH (1.5) | >91.6 | 100 | >85.7 | 100 |
| Intestinal pH (7.4) | >79.4 | 50.8* | 45.4* | 30.8* |
| Alveolar pH (7.4) | >68 | >59.6 | 35.4* | 26.1* |
| Interstitial pH (7.4) | 78.4 | >80.4 | 40* | 43.1* |
| Serum | >85 | >66.9 | 42.9* | 46.6* |
| Intracellular pH (4.5) | >89.6 | 100 | >79.1 | >78.1 |

* maximum extraction level at 72 hours

All data is taken from Stopford et al. (unpublished) Bioequivalency Testing of Cobalt Compounds. Conducted by Duke University Medical Center, Division of Occupational and Environmental Medicine for the Cobalt Development Institute.

**Table 2: Summary of Data for Aluminum Stearates and Dissociation Products**

| **Compound** | **Physical Chemical Properties** | | | |
|---|---|---|---|---|
| | Melting Point (deg C) | Boiling Point (deg C) | Vapor Pressure (hPa) | Water Solubility (g/L) |
| Aluminum Distearate | 145 | - | - | Not water soluble |
| Aluminum Tristearate | 100-120 | Decomposes | - | Not water soluble |
| *Dissociation Product:* Aluminum chloride | 190 | 182 | 1.38 @ 100 deg C | 450 @ 20 deg C |
| *Dissociation Product:* Stearic acid | 69-70 | 383 | 1.33 @174 | .00568 @25 deg C |

**Table 2 (continued): Summary of Data for Aluminum Stearates and Dissociation Products**

| **Compound** | **Environmental Fate** | | | | |
|---|---|---|---|---|---|
| | Partition Coefficient | Stability in Water | Photodegradation | Level III Fugacity Model | Biodegradation |
| Aluminum Distearate | - (not soluble in water) | - (not soluble in water) | .248 days | Air: 0.126<br>Water: 3.35<br>Soil: 30<br>Sediment: 66.5 | - (not soluble in water) |
| Aluminum Tristearate | - (not soluble in water) | - (not soluble in water) | .2 days | Air 0.0598<br>Water 2.35<br>Soil 29.9<br>Sediment 67.7 | - (not soluble in water) |
| *Dissociation Product:* Aluminum chloride | 1.26 (calc) | Unstable | - | Air: 5.39E-006<br>Water: 39.8<br>Soil: 60.1<br>Sediment: 0.0767 | - |
| *Dissociation Product:* Stearic acid | 8.42 | - (low water solubility) | T ½ = .5 days | Air: 0.676<br>Water: 7.19<br>Soil: 28.9<br>Sediment: 63.3 | Readily biodegradable |

**Table 2 (continued): Summary of Data for Aluminum Stearates and Dissociation Products**

| **Compound** | **Environmental Effects** | | | |
|---|---|---|---|---|
| | Acute Toxicity to Fish (mg/L) | Acute Toxicity to Daphnia (mg/L) | Acute Toxicity to Algae (mg/L) | Chronic Toxicity to Daphnia (mg/L) |
| Aluminum Distearate | - (not soluble in water) | - (not soluble in water) | - (not soluble in water) | 14- and 21-d EC50 (immobilization) = 0.24 and 0.048 mg/L; 21-d EC50 (reproduction) = 0.059 mg/L. LOEC = 0.020 mg/L; NOEC = 0.0061 mg/L. |
| Aluminum Tristearate | - (not soluble in water) | - (not soluble in water) | - (not soluble in water) | - |
| *Dissociation Product:* Aluminum chloride | 96 hr LC50 = 8.6 | 48 hr EC50=1.5 | - | - |
| *Dissociation Product:* Stearic acid | 96 hr = 12 | - | - | - |

**Table 2(continued): Summary of Available and Relevant Data for Aluminum Stearates and Dissociation Products**

| **Compound** | **Mammalian Toxicity** | | | | |
|---|---|---|---|---|---|
| | Acute Toxicity (mg/kg) | Repeat Dose Toxicity | Reproductive Effects | Developmental Effects | Genetic Toxicity |
| Aluminum Distearate | - | NOAEL (rat) = 1000 mg/kg bw (7 days) | - | - | - |
| Aluminum Tristearate | - | - | - | - | - |
| Aluminum chloride | LD50 = 370 (rat) | NOAEL (mouse) = 195 (5 or 7 weeks) | NOAEL (3-gerneration reproductive study in mice) = 19.3 mg/kg/d | NOAEL (fetal toxicity; rat) = 75 mg/kg LOAEL (maternal toxicity; rat) = 75 mg/kg | Bacterial mutation =negative Mammalian cell mutation (in vitro or in vivo) = negative |
| Stearic acid | LD50 = 4600 (rat) | 50 g/kg/d for 24 weeks produced reversible lipogranulomas | - | - | - |

# APPENDIX A

# ALUMINUM CHLORIDE ROBUST SUMMARIES

# APPENDIX B
# STEARIC ACID ROBUST SUMMARIES

# APPENDIX C
# ALUMNIMUM DISTEARATE ROBUST SUMMARIES

# APPENDIX D
# ALUMNIMUM TRISTEARATE ROBUST SUMMARIES